

APPENDIX B

SCREENING TABLES AND REFERENCE VALUES

FOR THE WATER PATHWAY

Note: The following exhibits are provided using K_{ow} values from the *DEA* (U.S. EPA, 1992a). EPA is currently revising criteria for selecting K_{ow} values, and these exhibits will be updated with appropriate K_{ow} values, as well as expanded to include more chemicals. The new changes may also affect Equation 3.8 and all other related evaluations.

EXHIBIT B-1**FLYNN DATA SET**Notes:

1. The predicted K_p was calculated using Equation 3.8 using the Lotus spreadsheet software, and is the average value of the regression correlation equation.
2. 95% LCL (lower confidence level) and UCL (upper confidence level) of K_p are calculated using the statistical software package STATA (STATA Corporation, 702 University Drive East, College Station, Texas 77840, USA).
3. Compounds in italics are common to both the Flynn data set and the organic data set. For these compounds, the 95% LCL and UCL are obtained from Exhibit B-1 and are common to both Exhibits B-1 and B-2.

| | Flynn's <i>in vitro</i> experimental data | MW | Log K_{ow} | K_p 95% LCL | K_p Predicted (cm/hr) | K_p Measured (<i>in vitro</i> data) cm/hr | K_p 95% UCL |
|----|---|-----------|---------------------------|------------------------------|--|--|------------------------------|
| 1 | Aldosterone | 360.4 | 1.08 | 4.4E-05 | 7.8E-05 | 3.0E-06 | 1.4E-04 |
| 2 | Amobarbital | 226.3 | 1.96 | 1.2E-03 | 1.7E-03 | 2.3E-03 | 2.4E-03 |
| 3 | Atropine | 289.4 | 1.81 | 4.1E-04 | 5.9E-04 | 8.5E-06 | 8.6E-04 |
| 4 | Barbital | 184.2 | 0.65 | 2.4E-04 | 3.9E-04 | 1.1E-04 | 6.4E-04 |
| 5 | Benzyl alcohol | 108.1 | 1.10 | 1.3E-03 | 2.1E-03 | 6.0E-03 | 3.4E-03 |
| 6 | <i>4-Bromophenol</i> | 173 | 2.59 | 5.8E-03 | 8.8E-03 | 3.6E-02 | 1.3E-02 |
| 7 | <i>2,3-Butanediol</i> | 90.12 | -0.92 | 5.2E-05 | 1.2E-04 | 4.0E-05 | 2.8E-04 |
| 8 | Butanoic acid (butyric acid) | 88.1 | 0.79 | 9.9E-04 | 1.7E-03 | 1.0E-03 | 2.9E-03 |
| 9 | <i>n-Butanol</i> | 74.12 | 0.88 | 1.3E-03 | 2.3E-03 | 2.5E-03 | 4.0E-03 |
| 10 | 2-Butanone | 72.1 | 0.28 | 5.1E-04 | 9.5E-04 | 4.5E-03 | 1.8E-03 |
| 11 | Butobarbital | 212.2 | 1.65 | 8.8E-04 | 1.3E-03 | 1.9E-04 | 1.8E-03 |
| 12 | <i>4-Chlorocresol</i> | 142.6 | 3.10 | 1.7E-02 | 2.9E-02 | 5.5E-02 | 4.9E-02 |
| 13 | <i>2-Chlorophenol</i> | 128.6 | 2.15 | 5.2E-03 | 8.0E-03 | 3.3E-02 | 1.2E-02 |
| 14 | <i>4-Chlorophenol</i> | 128.6 | 2.39 | 7.3E-03 | 1.2E-02 | 3.6E-02 | 1.8E-02 |
| 15 | Chloroxylenol | 156.6 | 3.39 | 2.1E-02 | 3.7E-02 | 5.2E-02 | 6.6E-02 |
| 16 | Codeine | 299.3 | 0.89 | 7.6E-05 | 1.3E-04 | 4.9E-05 | 2.2E-04 |
| 17 | Cortexolone (11-desoxy-17-hydroxycorticosterone) | 346.4 | 2.52 | 5.6E-04 | 8.4E-04 | 7.4E-05 | 1.3E-03 |
| 18 | Cortexone (deoxycorticosterone) | 330.4 | 2.88 | 1.2E-03 | 1.8E-03 | 4.5E-04 | 2.7E-03 |
| 19 | Corticosterone | 346.4 | 1.94 | 2.2E-04 | 3.5E-04 | 6.0E-05 | 5.4E-04 |
| 20 | Cortisone | 360.5 | 1.42 | 7.7E-05 | 1.3E-04 | 1.0E-05 | 2.2E-04 |
| 21 | <i>o-Cresol</i> | 108.1 | 1.95 | 4.8E-03 | 7.7E-03 | 1.6E-02 | 1.2E-02 |
| 22 | <i>m-Cresol</i> | 108.1 | 1.96 | 4.9E-03 | 7.8E-03 | 1.5E-02 | 1.2E-02 |
| 23 | <i>p-Cresol</i> | 108.1 | 1.95 | 4.8E-03 | 7.7E-03 | 1.8E-02 | 1.2E-02 |

EXHIBIT B-1**FLYNN DATA SET (continued)**

| | Flynn's <i>in vitro</i> experimental data | MW | Log K_{ow} | K_p 95% LCL | K_p Predicted (cm/hr) | K_p Measured (<i>in vitro</i> data) cm/hr | K_p 95% UCL |
|----|--|-----------|---------------------------|--------------------------------------|--|--|--------------------------------------|
| 24 | <i>n-Decanol</i> | 158.3 | 4.57 | 9.5E-02 | 2.2E-01 | 7.9E-02 | 5.1E-01 |
| 25 | <i>2,4-Dichlorophenol</i> | 163 | 3.06 | 1.2E-02 | 2.1E-02 | 6.0E-02 | 3.4E-02 |
| 26 | Digitoxin | 764.9 | 1.86 | 3.5E-07 | 1.4E-06 | 1.3E-05 | 5.4E-06 |
| 27 | Ephedrine | 165.2 | 1.03 | 5.8E-04 | 9.0E-04 | 6.0E-03 | 1.4E-03 |
| 28 | B-estradiol | 272.4 | 2.69 | 2.0E-03 | 2.8E-03 | 3.0E-04 | 4.1E-03 |
| 29 | B-estradiol (2) | 272.4 | 2.69 | 2.0E-03 | 2.8E-03 | 5.2E-03 | 4.1E-03 |
| 30 | Estriol | 288.4 | 2.47 | 1.2E-03 | 1.7E-03 | 4.0E-05 | 2.4E-03 |
| 31 | Estrone | 270.4 | 2.76 | 2.2E-03 | 3.3E-03 | 3.6E-03 | 4.7E-03 |
| 32 | <i>Ethanol</i> | 46.07 | -0.31 | 2.6E-04 | 5.4E-04 | 7.9E-04 | 1.1E-03 |
| 33 | <i>2-Ethoxy ethanol (Cellosolve)</i> | 90.12 | -0.32 | 1.5E-04 | 3.0E-04 | 2.5E-04 | 6.1E-04 |
| 34 | <i>Ethyl ether</i> | 74.12 | 0.89 | 1.4E-03 | 2.3E-03 | 1.6E-02 | 4.0E-03 |
| 35 | <i>4-Ethylphenol</i> | 122.2 | 2.58 | 1.0E-02 | 1.7E-02 | 3.5E-02 | 2.7E-02 |
| 36 | Etorphine | 411.5 | 1.86 | 7.6E-05 | 1.3E-04 | 3.6E-03 | 2.3E-04 |
| 37 | Fentanyl | 336.5 | 4.37 | 8.4E-03 | 1.6E-02 | 5.6E-03 | 3.2E-02 |
| 38 | Fentanyl (2) | 336.5 | 4.37 | 8.4E-03 | 1.6E-02 | 1.0E-02 | 3.2E-02 |
| 39 | Fluocinonide | 494.6 | 3.19 | 1.8E-04 | 3.5E-04 | 1.7E-03 | 6.8E-04 |
| 40 | Heptanoic acid (enanthic acid) | 130.2 | 2.50 | 8.4E-03 | 1.3E-02 | 2.0E-02 | 2.1E-02 |
| 41 | <i>n-Heptanol</i> | 116.2 | 2.62 | 1.2E-02 | 1.9E-02 | 3.2E-02 | 3.2E-02 |
| 42 | Hexanoic acid (caproic acid) | 116.2 | 1.90 | 4.1E-03 | 6.4E-03 | 1.4E-02 | 1.0E-02 |
| 43 | <i>n-Hexanol</i> | 102.2 | 2.03 | 5.8E-03 | 9.3E-03 | 1.3E-02 | 1.5E-02 |
| 44 | Hydrocortisone | 362.5 | 1.53 | 9.0E-05 | 1.5E-04 | 3.0E-06 | 2.5E-04 |
| 45 | Hydrocortisone (2) | 362.5 | 1.53 | 9.0E-05 | 1.5E-04 | 1.2E-04 | 2.5E-04 |
| 46 | [Hydrocortisone-21-yl]-N,N dimethyl succinamate | 489.6 | 2.03 | 3.1E-05 | 6.3E-05 | 6.8E-05 | 1.3E-04 |
| 47 | [Hydrocortisone-21-yl]-hemipimelate | 504.6 | 3.26 | 1.7E-04 | 3.4E-04 | 1.8E-03 | 6.8E-04 |
| 48 | [Hydrocortisone-21-hemisuccinate | 462.5 | 2.11 | 5.3E-05 | 1.0E-04 | 6.3E-04 | 1.9E-04 |
| 49 | [Hydrocortisone-21-yl]-hexanoate | 460.6 | 4.48 | 1.8E-03 | 3.9E-03 | 1.8E-02 | 8.2E-03 |
| 50 | [Hydrocortisone-21-yl]-6-hydroxy hexanoate | 476.6 | 2.79 | 1.3E-04 | 2.4E-04 | 9.1E-04 | 4.5E-04 |
| 51 | [Hydrocortisone-21-yl]-octanoate | 488.7 | 5.49 | 4.8E-03 | 1.3E-02 | 6.2E-02 | 3.3E-02 |
| 52 | [Hydrocortisone-21-yl]-pimelamate | 503.6 | 2.31 | 3.9E-05 | 8.0E-05 | 8.9E-04 | 1.6E-04 |
| 53 | [Hydrocortisone-21-yl]-propionate | 418.5 | 3.00 | 4.1E-04 | 6.9E-04 | 3.4E-03 | 1.2E-03 |
| 54 | [Hydrocortisone-21-yl]-succinamate | 461.6 | 1.43 | 1.8E-05 | 3.6E-05 | 2.6E-05 | 7.3E-05 |
| 55 | Hydromorphone | 285.3 | 1.25 | 1.7E-04 | 2.7E-04 | 1.5E-05 | 4.1E-04 |
| 56 | Hydroxypregnolone | 330.4 | 3.00 | 1.4E-03 | 2.2E-03 | 6.0E-04 | 3.3E-03 |
| 57 | 17a-Hydroxyprogesterone | 330.4 | 2.74 | 9.7E-04 | 1.5E-03 | 6.0E-04 | 2.2E-03 |
| 58 | Isoquinoline | 129.2 | 2.03 | 4.3E-03 | 6.6E-03 | 1.7E-02 | 1.0E-02 |

EXHIBIT B-1**FLYNN DATA SET (continued)**

| | Flynn's <i>in vitro</i> experimental data | MW | Log K_{ow} | K_p 95% LCL | K_p Predicted (cm/hr) | K_p Measured (<i>in vitro</i> data) cm/hr | K_p 95% UCL |
|----|--|-----------|---------------------------|--------------------------------------|--|--|--------------------------------------|
| 59 | Meperidine | 247 | 2.72 | 2.8E-03 | 4.1E-03 | 3.7E-03 | 6.0E-03 |
| 60 | <i>Methanol</i> | 32.04 | -0.77 | 1.4E-04 | 3.2E-04 | 5.0E-04 | 7.3E-04 |
| 61 | Methyl-[hydrocortisone-21-yl]-succinate | 476.6 | 2.58 | 9.1E-05 | 1.7E-04 | 2.1E-04 | 3.3E-04 |
| 62 | Methyl-[hydrocortisone-21-yl]-pimelate | 518.6 | 3.70 | 2.6E-04 | 5.5E-04 | 5.4E-03 | 1.2E-03 |
| 63 | <i>Methyl-4-hydroxy benzoate</i> | 152.1 | 1.96 | 3.0E-03 | 4.4E-03 | 9.1E-03 | 6.5E-03 |
| 64 | Morphine | 285.3 | 0.62 | 5.8E-05 | 1.0E-04 | 9.3E-06 | 1.8E-04 |
| 65 | <i>2-Naphthol</i> | 144.2 | 2.84 | 1.1E-02 | 1.9E-02 | 2.8E-02 | 3.1E-02 |
| 66 | Naproxen | 230.3 | 3.18 | 6.6E-03 | 1.0E-02 | 4.0E-04 | 1.6E-02 |
| 67 | Nicotine | 162.2 | 1.17 | 7.6E-04 | 1.2E-03 | 1.9E-02 | 1.8E-03 |
| 68 | Nitroglycerine | 227.1 | 2.00 | 1.3E-03 | 1.8E-03 | 1.1E-02 | 2.5E-03 |
| 69 | <i>3-Nitrophenol</i> | 139.1 | 2.00 | 3.7E-03 | 5.5E-03 | 5.6E-03 | 8.4E-03 |
| 70 | <i>4-Nitrophenol</i> | 139.1 | 1.91 | 3.2E-03 | 4.8E-03 | 5.6E-03 | 7.3E-03 |
| 71 | <i>n-Nonanol</i> | 144.3 | 3.77 | 4.0E-02 | 7.8E-02 | 6.0E-02 | 1.5E-01 |
| 72 | Octanoic acid (caprylic acid) | 144.2 | 3.00 | 1.4E-02 | 2.4E-02 | 2.5E-02 | 4.0E-02 |
| 73 | <i>n-Octanol</i> | 130.2 | 2.97 | 1.6E-02 | 2.7E-02 | 5.2E-02 | 4.7E-02 |
| 74 | Pentanoic acid (valeric acid) | 102.1 | 1.30 | 1.9E-03 | 3.1E-03 | 2.0E-03 | 4.9E-03 |
| 75 | <i>n-Pentanol</i> | 88.15 | 1.56 | 3.4E-03 | 5.5E-03 | 6.0E-03 | 8.9E-03 |
| 76 | Phenobarbital | 232.2 | 1.47 | 5.1E-04 | 7.4E-04 | 4.6E-04 | 1.1E-03 |
| 77 | <i>Phenol</i> | 94.11 | 1.46 | 2.7E-03 | 4.3E-03 | 8.1E-03 | 7.0E-03 |
| 78 | Pregnenolone | 316.5 | 3.13 | 2.0E-03 | 3.2E-03 | 1.5E-03 | 4.9E-03 |
| 79 | Progesterone | 314.4 | 3.77 | 5.0E-03 | 8.6E-03 | 1.5E-03 | 1.5E-02 |
| 80 | <i>n-Propanol</i> | 60.1 | 0.25 | 5.6E-04 | 1.1E-03 | 1.4E-03 | 2.0E-03 |
| 81 | <i>Resorcinol</i> | 110.1 | 0.80 | 7.7E-04 | 1.3E-03 | 2.4E-04 | 2.1E-03 |
| 82 | Salicylic acid | 138.1 | 2.26 | 5.4E-03 | 8.4E-03 | 6.3E-03 | 1.3E-02 |
| 83 | Scopolamine | 303.4 | 1.24 | 1.3E-04 | 2.1E-04 | 5.0E-05 | 3.3E-04 |
| 84 | Sucrose | 342.3 | -2.25 | 1.6E-07 | 6.0E-07 | 5.2E-06 | 2.3E-06 |
| 85 | Sufentanyl | 387.5 | 4.59 | 5.7E-03 | 1.2E-02 | 1.2E-02 | 2.4E-02 |
| 86 | Testosterone | 288.4 | 3.31 | 3.8E-03 | 6.0E-03 | 4.0E-04 | 9.4E-03 |
| 87 | <i>Thymol</i> | 150.2 | 3.34 | 2.1E-02 | 3.7E-02 | 5.2E-02 | 6.6E-02 |
| 88 | <i>2,4,6-Trichlorophenol</i> | 197.4 | 3.69 | 1.9E-02 | 3.5E-02 | 5.9E-02 | 6.2E-02 |
| 89 | Water | 18.01 | -1.38 | 5.8E-05 | 1.5E-04 | 5.0E-04 | 3.9E-04 |
| 90 | <i>3,4-Xylenol</i> | 122.2 | 2.35 | 7.4E-03 | 1.2E-02 | 3.6E-02 | 1.9E-02 |

EXHIBIT B-2**PREDICTED K_p FOR ORGANIC CONTAMINANTS IN WATER**Notes:

1. Chemicals with an asterisk (*) preceding them have been identified to be outside the effective prediction domain (EPD). EPD determination is calculated using the software package MLAB (Civilized Software, Inc., 8120 Woodmont Avenue, #250, Bethesda, MD 20814, USA).
2. Chemicals with two asterisks (**) are halogenated compounds. Because halogenated chemicals have a lower ratio of molar volume relative to their molecular weight than hydrocarbons (due to the relatively weighty halogen atom), the K_p correlation based on molecular weight of hydrocarbons will tend to underestimate permeability coefficients for halogenated organic chemicals. To address this problem, a new K_p correlation based on molar volume and log K_{ow} will be explored. In selecting the halogenated compounds, the focus was on trihalomethanes, the halogenated acids, and the halogenated aliphatics with halogenated molecules contributing to a large percentage of the molecular weight.
3. K_p is obtained from the modified Potts and Guy's equation (Equation 3.8). Values in the exhibit are obtained from the organic spreadsheet (ORG04_01.WK4) where the coefficients of Equation 3.8 carry more significant figures than shown in Chapter 3 and Appendix A.
4. 95% LCL and UCL are calculated using the statistical software package STATA (STATA Corporation, 702 University Drive East, College Station, Texas 77840, USA). Compounds in italics are common to both the Flynn data set and the organic data set. For these compounds, the 95% LCL and UCL are obtained from Exhibit B-1 and common to both Exhibits B-1 and B-2.
5. All calculations are performed using the Lotus spreadsheet software, except where noted.

| | CHEMICAL | CAS No. | MW | log K_{ow} | K_p 95% LCL | K_p (cm/hr) predicted | K_p (cm/hr) measured | K_p 95% UCL |
|------|---------------------------------|----------------|-----------|---------------------------|--------------------------------------|--|---|----------------------------------|
| 1 | Acetaldehyde | 75070 | 44.1 | -0.22 | 2.4E-05 | 6.3E-04 | | 1.6E-02 |
| 2 | Acetamide | 60355 | 59 | -1.26 | 3.9E-06 | 1.1E-04 | | 2.9E-03 |
| 3 | Acetylaminofluorene, 2- | 53963 | 223 | 3.24 | 5.0E-04 | 1.2E-02 | | 3.1E-01 |
| 4 | Acrolein | 107028 | 56.1 | -0.10 | 2.5E-05 | 6.5E-04 | | 1.7E-02 |
| 5 | Acrylamide | 79061 | 71 | -0.67 | 8.5E-06 | 2.2E-04 | | 5.9E-03 |
| 6 | Acrylonitrile | 107131 | 53.1 | 0.25 | 4.5E-05 | 1.2E-03 | | 2.9E-02 |
| 7 | Aldrin | 309002 | 365 | 3.01 | 5.7E-05 | 1.4E-03 | | 3.5E-02 |
| ** 8 | Allyl chloride | 107051 | 76.5 | 1.45 | 2.2E-04 | 5.4E-03 | | 1.3E-01 |
| 9 | Amino-2-methylanthraquinone, 1- | 82280 | 237.3 | 2.80 | 2.2E-04 | 5.3E-03 | | 1.3E-01 |
| 10 | Aminoanthraquinone, 2- | 117793 | 223 | 2.15 | 9.7E-05 | 2.4E-03 | | 5.7E-02 |
| 11 | Aminoazobenzene, p- | 60093 | 197 | 2.62 | 2.8E-04 | 6.8E-03 | | 1.7E-01 |
| 12 | Aminoazotoluene, o- | 97563 | 225.3 | 3.92 | 1.4E-03 | 3.4E-02 | | 8.7E-01 |
| 13 | Aminobiphenyl, 4- | 92671 | 169.2 | 2.80 | 5.2E-04 | 1.3E-02 | | 3.2E-01 |

EXHIBIT B-2**PREDICTED K_p FOR ORGANIC CONTAMINANTS IN WATER (continued)**

| | CHEMICAL | CAS No. | MW | log K _{ow} | K _p 95% LCL | K _p (cm/hr) predicted | K _p (cm/hr) measured | K _p 95% UCL |
|----|-------------------------|---------|-------|---------------------|------------------------------|--|---------------------------------------|---------------------------|
| 14 | Aniline | 62533 | 93.1 | 0.90 | 7.5E-05 | 1.9E-03 | | 4.7E-02 |
| 15 | Anisidine, o- | 90040 | 145 | 1.18 | 5.9E-05 | 1.5E-03 | | 3.6E-02 |
| 16 | Auramine | 492808 | 267.4 | 3.54 | 4.5E-04 | 1.1E-02 | | 2.8E-01 |
| 17 | Benzene | 71432 | 78.1 | 2.13 | 5.9E-04 | 1.5E-02 | | 3.7E-01 |
| 18 | Benzidine | 92875 | 184.2 | 1.34 | 4.6E-05 | 1.1E-03 | | 2.8E-02 |
| * | 19 Benzo-a-anthracene | 56553 | 228.3 | 5.66 | 1.7E-02 | 4.7E-01 | | 1.3E+01 |
| * | 20 Benzo-a-pyrene | 50328 | 250 | 6.10 | 2.4E-02 | 7.0E-01 | | 2.0E+01 |
| * | 21 Benzo-b-fluoranthene | 205992 | 252.3 | 6.12 | 2.4E-02 | 7.0E-01 | | 2.0E+01 |
| 22 | Benzoic acid | 65850 | 122 | 1.87 | 2.3E-04 | 5.7E-03 | | 1.4E-01 |
| 23 | Benzotrichloride | 98077 | 195 | 2.92 | 4.5E-04 | 1.1E-02 | | 2.7E-01 |
| 24 | Benzyl chloride | 100447 | 127 | 2.30 | 4.1E-04 | 1.0E-02 | | 2.5E-01 |
| 25 | Bis(2-chloroethyl)ether | 111444 | 143 | 1.29 | 7.2E-05 | 1.8E-03 | | 4.4E-02 |
| ** | 26 Bromodichloromethane | 75274 | 163.8 | 2.09 | 1.9E-04 | 4.6E-03 | | 1.1E-01 |
| ** | 27 Bromoform | 75252 | 252.8 | 2.37 | 9.2E-05 | 2.2E-03 | | 5.5E-02 |
| ** | 28 Bromomethane | 74839 | 95 | 1.19 | 1.1E-04 | 2.8E-03 | | 7.0E-02 |
| 29 | Bromophenol, p- | 106412 | 173 | 2.59 | 5.8E-03 | 8.8E-03 | | 1.3E-02 |
| 30 | Butadiene, 1,3- | 106990 | 54 | 1.99 | 6.5E-04 | 1.6E-02 | | 4.1E-01 |
| 31 | 2,3-Butanediol | 513859 | 90.12 | -0.92 | 5.2E-05 | 1.2E-04 | 4.0E-05 | 2.8E-04 |
| 32 | n-Butanol | 71363 | 74.12 | 0.88 | 1.3E-03 | 2.3E-03 | 2.5E-03 | 4.0E-03 |
| 33 | Butoxyethanol, 2- | 111762 | 118 | 0.83 | 4.9E-05 | 1.2E-03 | | 3.0E-02 |
| 34 | Captan | 133062 | 300 | 2.35 | 4.8E-05 | 1.2E-03 | | 2.9E-02 |
| 35 | Carbon disulfide | 75150 | 80 | 2.24 | 6.9E-04 | 1.7E-02 | | 4.3E-01 |
| ** | 36 Carbon tetrachloride | 56235 | 153.8 | 2.83 | 6.6E-04 | 1.6E-02 | | 4.0E-01 |
| 37 | Chlordane | 57749 | 409.8 | 5.54 | 1.4E-03 | 3.8E-02 | | 1.0E+00 |
| 38 | Chlordane (cis) | 5103719 | 410 | 5.47 | 1.2E-03 | 3.4E-02 | | 9.2E-01 |
| 39 | Chlordane (trans) | 5103742 | 410 | 5.47 | 1.2E-03 | 3.4E-02 | | 9.2E-01 |
| 40 | Chlorobenzene | 108907 | 112.6 | 2.84 | 1.1E-03 | 2.8E-02 | | 7.1E-01 |
| 41 | 4-Chlorocresol | 59507 | 142.6 | 3.10 | 1.7E-02 | 2.9E-02 | 5.5E-02 | 4.9E-02 |
| ** | 42 Chlorodibromomethane | 124481 | 208.3 | 2.23 | 1.3E-04 | 3.2E-03 | | 7.9E-02 |
| ** | 43 Chloroethane | 75003 | 64.5 | 1.43 | 2.4E-04 | 6.1E-03 | | 1.5E-01 |
| ** | 44 Chloroform | 67663 | 119.4 | 1.97 | 2.8E-04 | 6.8E-03 | | 1.7E-01 |
| ** | 45 Chloromethane | 74873 | 50.5 | 0.91 | 1.3E-04 | 3.3E-03 | | 8.3E-02 |
| 46 | 2-Chlorophenol | 95578 | 128.6 | 2.15 | 5.2E-03 | 8.0E-03 | 3.3E-02 | 1.2E-02 |
| 47 | 4-Chlorophenol | 106489 | 128.6 | 2.39 | 7.3E-03 | 1.2E-02 | 3.6E-02 | 1.8E-02 |
| 48 | Chlorothalonil | 1897456 | 265.9 | 3.86 | 7.4E-04 | 1.9E-02 | | 4.7E-01 |
| * | 49 Chrysene | 218019 | 228.3 | 5.66 | 1.7E-02 | 4.7E-01 | | 1.3E+01 |
| 50 | Cresidine, p- | 120718 | 137.2 | 1.67 | 1.4E-04 | 3.4E-03 | | 8.4E-02 |
| 51 | m-Cresol | 108394 | 108.1 | 1.96 | 4.9E-03 | 7.8E-03 | 1.5E-02 | 1.2E-02 |
| 52 | o-Cresol | 95487 | 108.1 | 1.95 | 4.8E-03 | 7.7E-03 | 1.6E-02 | 1.2E-02 |

EXHIBIT B-2**PREDICTED K_p FOR ORGANIC CONTAMINANTS IN WATER (continued)**

| | CHEMICAL | CAS No. | MW | log K _{ow} | K _p 95% LCL | K _p (cm/hr) predicted | K _p (cm/hr) measured | K _p 95% UCL |
|----|--------------------------------|---------|-------|---------------------|------------------------------|--|---------------------------------------|---------------------------|
| 53 | <i>p</i> -Cresol | 106445 | 108.1 | 1.95 | 4.8E-03 | 7.7E-03 | 1.8E-02 | 1.2E-02 |
| * | DDD | 72548 | 320 | 5.80 | 6.4E-03 | 1.8E-01 | | 5.0E+00 |
| * | DDE | 72559 | 318 | 5.69 | 5.6E-03 | 1.6E-01 | | 4.3E+00 |
| * | DDT | 50293 | 355 | 6.36 | 9.2E-03 | 2.7E-01 | | 7.8E+00 |
| * | <i>n</i> -Decanol | 112301 | 158.3 | 4.57 | 9.5E-02 | 2.2E-01 | 7.9E-02 | 5.1E-01 |
| 58 | Di-2-ethylhexyl phthalate | 117817 | 391 | 5.11 | 9.4E-04 | 2.5E-02 | | 6.6E-01 |
| 59 | Diaminoanisole, 2,4- | 615054 | 138.2 | -0.12 | 8.5E-06 | 2.2E-04 | | 5.6E-03 |
| 60 | Diaminotoluene | 95807 | 122 | 0.34 | 2.2E-05 | 5.4E-04 | | 1.4E-02 |
| 61 | Diaminotoluene, 2,4- | 101804 | 200 | 2.06 | 1.1E-04 | 2.8E-03 | | 6.7E-02 |
| * | Dibenzo(a,h)anthracene | 53703 | 278.4 | 6.84 | 4.9E-02 | 1.5E+00 | | 4.7E+01 |
| 63 | Dibutyl phthalate | 84742 | 278 | 4.13 | 9.4E-04 | 2.4E-02 | | 6.1E-01 |
| 64 | Dichlorobenzene, 1,2- | 95501 | 147 | 3.38 | 1.6E-03 | 4.1E-02 | | 1.0E+00 |
| 65 | Dichlorobenzene, 1,3- | 541731 | 147 | 3.60 | 2.3E-03 | 5.8E-02 | | 1.5E+00 |
| 66 | Dichlorobenzene, 1,4- | 106467 | 147 | 3.39 | 1.7E-03 | 4.2E-02 | | 1.1E+00 |
| 67 | Dichlorobenzidine, 3,3' | 91941 | 253.1 | 3.51 | 5.1E-04 | 1.3E-02 | | 3.2E-01 |
| ** | Dichlorodifluoromethane | 75718 | 120.9 | 2.16 | 3.6E-04 | 9.0E-03 | | 2.2E-01 |
| ** | Dichloroethane, 1,1- | 75343 | 99 | 1.79 | 2.7E-04 | 6.7E-03 | | 1.7E-01 |
| ** | Dichloroethane, 1,2- | 107062 | 99 | 1.48 | 1.7E-04 | 4.2E-03 | | 1.0E-01 |
| ** | Dichloroethylene, 1,1- | 75354 | 96.9 | 2.13 | 4.7E-04 | 1.2E-02 | | 2.9E-01 |
| ** | Dichloroethylene, 1,2- (trans) | 540590 | 96.9 | 1.86 | 3.1E-04 | 7.7E-03 | | 1.9E-01 |
| 73 | 2,4-Dichlorophenol | 120832 | 163 | 3.06 | 1.2E-02 | 2.1E-02 | 6.0E-02 | 3.4E-02 |
| ** | Dichloropropane, 1,2- | 78875 | 113 | 2.00 | 3.1E-04 | 7.8E-03 | | 1.9E-01 |
| ** | Dichloropropene, 1,3- | 542756 | 111 | 1.60 | 1.7E-04 | 4.3E-03 | | 1.1E-01 |
| 76 | Dichlorvos | 62737 | 221 | 1.47 | 3.5E-05 | 8.5E-04 | | 2.1E-02 |
| 77 | Dieldrin | 60571 | 381 | 4.56 | 4.7E-04 | 1.2E-02 | | 3.2E-01 |
| 78 | Diepoxybutane | 1464535 | 86.1 | -1.84 | 1.1E-06 | 3.1E-05 | | 8.7E-04 |
| 79 | Diethyl phthalate | 84662 | 222 | 2.47 | 1.6E-04 | 3.9E-03 | | 9.5E-02 |
| 80 | Diethyl sulfate | 64675 | 154 | 1.14 | 5.0E-05 | 1.2E-03 | | 3.0E-02 |
| 81 | Dimethoxybenzidine, 3,3'- | 119904 | 254.4 | 1.81 | 3.8E-05 | 9.3E-04 | | 2.3E-02 |
| 82 | Dimethyl phthalate | 131113 | 194 | 1.56 | 5.7E-05 | 1.4E-03 | | 3.4E-02 |
| 83 | Dimethyl sulfate | 77781 | 126 | 1.16 | 7.3E-05 | 1.8E-03 | | 4.5E-02 |
| 84 | Dimethylamine, n-nitroso- | 62759 | 74.1 | -0.57 | 9.6E-06 | 2.5E-04 | | 6.6E-03 |
| 85 | Dimethylaminoazobenzene, 4- | 60117 | 225 | 4.58 | 3.6E-03 | 9.5E-02 | | 2.5E+00 |
| 86 | Dimethylbenzidine, 3,3'- | 119937 | 212.3 | 2.34 | 1.5E-04 | 3.6E-03 | | 8.8E-02 |
| 87 | Dimethylcarbamyl chloride | 79447 | 107.5 | 0.00 | 4.9E-06 | 3.9E-04 | | 3.4E-03 |
| 88 | Dimethylhydrazine, 1,1- | 57147 | 60 | -1.50 | 2.6E-06 | 7.3E-05 | | 2.0E-03 |
| 89 | Dimethylphenol, 2,4- | 105679 | 122.2 | 2.30 | 4.4E-04 | 1.1E-02 | | 2.7E-01 |
| 90 | Dimethylphenol, 3,4- | 95658 | 122 | 2.23 | 4.0E-04 | 9.8E-03 | | 2.4E-01 |
| 91 | Dinitrophenol, 2,4- | 51285 | 184.1 | 1.54 | 6.3E-05 | 1.5E-03 | | 3.7E-02 |

EXHIBIT B-2**PREDICTED K_P FOR ORGANIC CONTAMINANTS IN WATER (continued)**

| | CHEMICAL | CAS No. | MW | log K _{ow} | K _p 95% LCL | K _p (cm/hr) predicted | K _p (cm/hr) measured | K _p 95% UCL |
|--------|-------------------------------|---------|-------|---------------------|------------------------------|--|---------------------------------------|---------------------------|
| 92 | Dinitrotoluene, 2,4- | 121142 | 182.1 | 1.98 | 1.3E-04 | 3.1E-03 | | 7.5E-02 |
| 93 | Dinitrotoluene, 2,6- | 606202 | 182.1 | 1.72 | 8.5E-05 | 2.1E-03 | | 5.1E-02 |
| 94 | Dioxane, 1,4- | 123911 | 88.1 | -0.27 | 1.3E-05 | 3.3E-04 | | 8.6E-03 |
| 95 | Diphenylamine, n-nitroso- | 86306 | 198.2 | 3.13 | 5.9E-04 | 1.5E-02 | | 3.6E-01 |
| 96 | Diphenylhydrazine, 1,2- | 122667 | 184.2 | 2.94 | 5.3E-04 | 1.3E-02 | | 3.2E-01 |
| 97 | Dipropylamine, n-nitroso- | 621647 | 130.2 | 1.36 | 9.5E-05 | 2.3E-03 | | 5.8E-02 |
| 98 | Endrin | 72208 | 381 | 4.56 | 4.7E-04 | 1.2E-02 | | 3.2E-01 |
| 99 | Epichlorohydrin | 106898 | 92 | -0.21 | 1.3E-05 | 3.5E-04 | | 8.9E-03 |
| 100 | Ethanol | 64175 | 46.07 | -0.31 | 2.6E-04 | 5.4E-04 | 7.9E-04 | 1.1E-03 |
| 101 | Ethanol, 2-(2-butoxyethoxy)- | 112345 | 162 | -0.92 | 1.8E-06 | 4.7E-05 | | 1.3E-03 |
| 102 | Ethanol, 2-(2-ethoxyethoxy)- | 111900 | 134 | -0.08 | 9.6E-06 | 2.5E-04 | | 6.3E-03 |
| 103 | Ethanol, 2-(2-methoxyethoxy)- | 111773 | 120 | -0.42 | 6.7E-06 | 1.7E-04 | | 4.5E-03 |
| 104 | 2-Ethoxy ethanol (Cellosolve) | 110805 | 90.12 | -0.32 | 1.5E-04 | 3.0E-04 | | 6.1E-04 |
| 105 | Ethoxyethyl acetate, 2- | 111159 | 132 | 0.65 | 3.1E-05 | 7.7E-04 | | 1.9E-02 |
| 106 | Ethyl acrylate | 140885 | 100 | 1.32 | 1.3E-04 | 3.2E-03 | | 8.0E-02 |
| 107 | Ethyl carbamate | 51796 | 89 | -0.15 | 1.5E-05 | 3.9E-04 | | 1.0E-02 |
| 108 | Ethyl ether | 60297 | 74.12 | 0.89 | 1.4E-03 | 2.3E-03 | 1.6E-02 | 4.0E-03 |
| 109 | Ethylbenzene | 100414 | 106.2 | 3.15 | 1.9E-03 | 4.9E-02 | | 1.2E+00 |
| 110 | Ethylene oxide | 75218 | 44.1 | -0.30 | 2.2E-05 | 5.6E-04 | | 1.5E-02 |
| ** 111 | Ethylenedibromide | 106934 | 188 | 1.96 | 1.1E-04 | 2.8E-03 | | 6.8E-02 |
| 112 | Ethyleneimine | 151564 | 43 | -1.12 | 6.0E-06 | 1.6E-04 | | 4.4E-03 |
| 113 | Ethylenethiourea | 96457 | 96 | -0.66 | 6.3E-06 | 1.7E-04 | | 4.3E-03 |
| 114 | 4-Ethylphenol | 123079 | 122.2 | 2.58 | 1.0E-02 | 1.7E-02 | 3.5E-02 | 2.7E-02 |
| * 115 | Fluoranthene | 206440 | 202.3 | 4.95 | 8.3E-03 | 2.2E-01 | | 6.0E+00 |
| 116 | Formaldehyde | 50000 | 30 | 0.35 | 7.1E-05 | 1.8E-03 | | 4.6E-02 |
| 117 | Glycerol | 56815 | 92.1 | -1.76 | 1.1E-06 | 3.2E-05 | | 9.1E-04 |
| 118 | Heptachlor | 76448 | 373.5 | 4.27 | 3.4E-04 | 8.6E-03 | | 2.2E-01 |
| 119 | n-Heptanol | 111706 | 116.2 | 2.62 | 1.2E-02 | 1.9E-02 | 3.2E-02 | 3.2E-02 |
| * 120 | Hexachlorobenzene | 118741 | 284.8 | 5.31 | 4.9E-03 | 1.3E-01 | | 3.6E+00 |
| ** 121 | Hexachlorobutadiene | 87683 | 260.8 | 4.78 | 3.1E-03 | 8.1E-02 | | 2.1E+00 |
| ** 122 | Hexachloroethane | 67721 | 236.7 | 3.93 | 1.2E-03 | 3.0E-02 | | 7.6E-01 |
| 123 | Hexamethylphosphoramide | 680319 | 179 | 0.03 | 6.4E-06 | 1.6E-04 | | 4.1E-03 |
| 124 | n-Hexanol | 111273 | 102.2 | 2.03 | 5.8E-03 | 9.3E-03 | 1.3E-02 | 1.5E-02 |
| * 125 | Hydrazine/Hydrazine sulfate | 302012 | 32 | -2.07 | 1.5E-06 | 4.4E-05 | | 1.3E-03 |
| * 126 | Indeno(1,2,3-CD)pyrene | 193395 | 276.3 | 6.58 | 3.5E-02 | 1.0E+00 | | 3.1E+01 |
| 127 | Isophorone | 78591 | 138.2 | 1.67 | 1.4E-04 | 3.4E-03 | | 8.3E-02 |
| 128 | Lindane | 58899 | 291 | 3.72 | 4.3E-04 | 1.1E-02 | | 2.7E-01 |
| 129 | Mechlorethamine | 51752 | 156 | 1.07 | 4.4E-05 | 1.1E-03 | | 2.6E-02 |
| 130 | Methanol | 67561 | 32.04 | -0.77 | 1.4E-04 | 3.2E-04 | 5.0E-04 | 7.3E-04 |

EXHIBIT B-2**PREDICTED K_p FOR ORGANIC CONTAMINANTS IN WATER (continued)**

| | CHEMICAL | CAS No. | MW | log K _{ow} | K _p 95% LCL | K _p (cm/hr) predicted | K _p (cm/hr) measured | K _p 95% UCL |
|--------|--|----------|-------|---------------------|------------------------------|--|---------------------------------------|---------------------------|
| 131 | Methoxyethanol, 2- | 109864 | 76 | -0.77 | 6.8E-06 | 1.8E-04 | | 4.8E-03 |
| 132 | Methoxypropan-2-ol, 1- | 107982 | 90 | -0.18 | 1.4E-05 | 3.7E-04 | | 9.6E-03 |
| 133 | Methyl ethyl ketone | 78933 | 72 | 0.29 | 3.8E-05 | 9.6E-04 | | 2.4E-02 |
| 134 | <i>Methyl-4-hydroxy benzoate</i> | 99763 | 152.1 | 1.96 | 3.0E-03 | 4.4E-03 | 9.1E-03 | 6.5E-03 |
| ** 135 | Methyl iodide | 74884 | 142 | 1.51 | 1.0E-04 | 2.5E-03 | | 6.2E-02 |
| 136 | Methylaziridine, 2- | 75558 | 57 | -0.60 | 1.1E-05 | 3.0E-04 | | 7.9E-03 |
| 137 | Methylene bis(2-chloroaniline), 4,4'- | 101144 | 267.2 | 3.94 | 8.2E-04 | 2.1E-02 | | 5.2E-01 |
| 138 | Methylene bis(N,N'-dimethyl)aniline, 4,4'- | 101611 | 254 | 4.75 | 3.2E-03 | 8.4E-02 | | 2.2E+00 |
| ** 139 | Methylene chloride | 75092 | 84.9 | 1.25 | 1.4E-04 | 3.5E-03 | | 8.8E-02 |
| 140 | Methylenedianiline, 4,4'- | 101779 | 198 | 1.59 | 5.7E-05 | 1.4E-03 | | 3.4E-02 |
| 141 | Michler's ketone | 90948 | 268.4 | 4.07 | 9.8E-04 | 2.5E-02 | | 6.3E-01 |
| ** 142 | Mustard Gas | 505602 | 159.1 | 2.03 | 1.8E-04 | 4.5E-03 | | 1.1E-01 |
| 143 | Naphthalene | 91203 | 128.2 | 3.30 | 1.8E-03 | 4.7E-02 | | 1.2E+00 |
| 144 | <i>2-Naphthol</i> | 135193 | 144.2 | 2.84 | 1.1E-02 | 1.9E-02 | 2.8E-02 | 3.1E-02 |
| 145 | Naphthylamine, 1- | 134327 | 143.2 | 2.25 | 3.1E-04 | 7.7E-03 | | 1.9E-01 |
| 146 | Naphthylamine, 2- | 91598 | 143.2 | 2.28 | 3.3E-04 | 8.1E-03 | | 2.0E-01 |
| 147 | Nitrolotriacetic acid | 139139 | 191 | -0.18 | 3.9E-06 | 1.0E-04 | | 2.6E-03 |
| 148 | Nitro-o-anisidine, 5- | 99592 | 152.7 | 1.47 | 8.4E-05 | 2.1E-03 | | 5.1E-02 |
| 149 | Nitrobiphenyl, 4- | 92933 | 199.2 | 3.77 | 1.5E-03 | 3.8E-02 | | 9.7E-01 |
| * 150 | Nitrofen | 1836755 | 284.1 | 5.53 | 6.8E-03 | 1.9E-01 | | 5.2E+00 |
| 151 | Nitrophenol, 2- | 88755 | 139.1 | 1.79 | 1.6E-04 | 4.0E-03 | | 9.9E-02 |
| 152 | Nitrophenol, 2-amino-4- | 99570 | 154.1 | 1.36 | 7.0E-05 | 1.7E-03 | | 4.2E-02 |
| 153 | <i>3-Nitrophenol</i> | 554847 | 139.1 | 2.00 | 3.7E-03 | 5.5E-03 | 5.6E-03 | 8.4E-03 |
| 154 | <i>4-Nitrophenol</i> | 100027 | 139.1 | 1.91 | 3.2E-03 | 4.8E-03 | 5.6E-03 | 7.3E-03 |
| 155 | Nitrophenol, 4-amino-2- | 119346 | 154.1 | 0.96 | 3.8E-05 | 9.3E-04 | | 2.3E-02 |
| 156 | Nitropropane, 2- | 79469 | 110 | 0.55 | 3.5E-05 | 8.8E-04 | | 2.2E-02 |
| 157 | Nitroso-di-n-butylamine, n- | 924163 | 158.2 | 1.92 | 1.6E-04 | 3.8E-03 | | 9.4E-02 |
| 158 | Nitroso-N-ethylurea, n- | 759739 | 117.1 | 0.23 | 1.9E-05 | 4.9E-04 | | 1.2E-02 |
| 159 | Nitroso-N-methylurea, n- | 684935 | 103.1 | -0.03 | 1.5E-05 | 3.9E-04 | | 1.0E-02 |
| 160 | Nitrosodiethanolamine, n- | 1116547 | 134 | -1.58 | 8.9E-07 | 2.5E-05 | | 6.9E-04 |
| 161 | Nitrosodiethylamine, n- | 55185 | 88 | 0.48 | 4.2E-05 | 1.0E-03 | | 2.6E-02 |
| 162 | Nitrosodiphenylamine, p- | 156105 | 198.2 | 3.50 | 1.0E-03 | 2.6E-02 | | 6.4E-01 |
| 163 | Nitrosomethylvinylamine, n- | 4549400 | 86.1 | 0.00 | 2.0E-05 | 5.1E-04 | | 1.3E-02 |
| 164 | Nitrosomorpholine, n- | 59892 | 116.1 | -0.44 | 6.9E-06 | 1.8E-04 | | 4.6E-03 |
| 165 | Nitrosonornicotine, n- | 16543558 | 177.2 | 0.03 | 6.5E-06 | 1.7E-04 | | 4.2E-03 |
| 166 | Nitrosopiperidine, n- | 100754 | 350.3 | 0.36 | 1.1E-06 | 2.9E-05 | | 7.6E-04 |
| 167 | <i>n-Nonanol</i> | 143088 | 144.3 | 3.77 | 4.0E-02 | 7.8E-02 | 6.0E-02 | 1.5E-01 |

EXHIBIT B-2**PREDICTED K_p FOR ORGANIC CONTAMINANTS IN WATER (continued)**

| | CHEMICAL | CAS No. | MW | log K _{ow} | K _p 95% LCL | K _p (cm/hr) predicted | K _p (cm/hr) measured | K _p 95% UCL |
|--------|------------------------------------|----------|-------|---------------------|------------------------------|--|---------------------------------------|---------------------------|
| 168 | <i>n-Octanol</i> | 111875 | 130.2 | 2.97 | 1.6E-02 | 2.7E-02 | 5.2E-02 | 4.7E-02 |
| 169 | Parathion | 56382 | 291 | 3.83 | 5.1E-04 | 1.3E-02 | | 3.2E-01 |
| * 170 | PCB-chlorobiphenyl, 4- | 2051629 | 292 | 6.50 | 2.5E-02 | 7.5E-01 | | 2.2E+01 |
| * 171 | PCB-hexachlorobiphenyl | 26601649 | 361 | 6.72 | 1.4E-02 | 4.3E-01 | | 1.3E+01 |
| ** 172 | Pentachloronitrobenzene | 82688 | 295.3 | 4.64 | 1.6E-03 | 4.2E-02 | | 1.1E+00 |
| * 173 | Pentachlorophenol | 87865 | 266.4 | 5.86 | 1.4E-02 | 3.9E-01 | | 1.1E+01 |
| 174 | <i>n-Pentanol</i> | 71410 | 88.15 | 1.56 | 3.4E-03 | 5.5E-03 | 6.0E-03 | 8.9E-03 |
| 175 | Pantanone, 4-methyl-2- | 108101 | 100 | 1.19 | 1.1E-04 | 2.7E-03 | | 6.6E-02 |
| * 176 | Phenanthrene | 85018 | 178.2 | 4.46 | 5.5E-03 | 1.4E-01 | | 3.8E+00 |
| 177 | <i>Phenol</i> | 108952 | 94.11 | 1.46 | 2.7E-03 | 4.3E-03 | 8.1E-03 | 7.0E-03 |
| 178 | Phenol, 4,6-dinitro-2-methyl- | 534521 | 198.1 | 2.12 | 1.3E-04 | 3.1E-03 | | 7.6E-02 |
| 179 | <i>n-Propanol</i> | 71238 | 60.1 | 0.25 | 5.6E-04 | 1.1E-03 | 1.4E-03 | 2.0E-03 |
| 180 | Propiolactone, beta- | 57578 | 72 | -0.46 | 1.2E-05 | 3.1E-04 | | 8.0E-03 |
| 181 | Propylene oxide | 75569 | 58.1 | 0.03 | 3.0E-05 | 7.7E-04 | | 2.0E-02 |
| 182 | <i>Resorcinol</i> | 108463 | 110.1 | 0.80 | 7.7E-04 | 1.3E-03 | 2.4E-04 | 2.1E-03 |
| 183 | Safrole | 94597 | 162.2 | 2.66 | 4.6E-04 | 1.1E-02 | | 2.8E-01 |
| 184 | Styrene | 100425 | 104.1 | 2.95 | 1.5E-03 | 3.7E-02 | | 9.4E-01 |
| 185 | Styrene oxide | 96093 | 120 | 1.61 | 1.6E-04 | 3.9E-03 | | 9.6E-02 |
| * 186 | TCDD | 1746016 | 322 | 6.80 | 2.7E-02 | 8.1E-01 | | 2.5E+01 |
| ** 187 | Tetrachlorethylene | 127184 | 165.8 | 3.40 | 1.3E-03 | 3.3E-02 | | 8.4E-01 |
| ** 188 | Tetrachloroethane, 1,1,2,2- | 79345 | 167.9 | 2.39 | 2.8E-04 | 6.9E-03 | | 1.7E-01 |
| 189 | Thioacetamide | 62555 | 75 | 0.71 | 7.0E-05 | 1.8E-03 | | 4.4E-02 |
| 190 | Thiodianiline, 4,4'- | 139651 | 216 | 2.03 | 8.8E-05 | 2.1E-03 | | 5.2E-02 |
| 191 | Thiourea | 62566 | 76 | -0.95 | 5.1E-06 | 1.4E-04 | | 3.7E-03 |
| 192 | <i>Thymol</i> | 89838 | 150.2 | 3.34 | 2.1E-02 | 3.7E-02 | 5.2E-02 | 6.6E-02 |
| 193 | Toluene | 108883 | 92.1 | 2.73 | 1.2E-03 | 3.1E-02 | | 7.8E-01 |
| 194 | Toluidine hydrochloride, o- | 636215 | 143.2 | 1.29 | 7.2E-05 | 1.8E-03 | | 4.4E-02 |
| 195 | Toluidine, o- | 95534 | 107 | 1.32 | 1.2E-04 | 3.0E-03 | | 7.3E-02 |
| 196 | Toxaphene | 8001352 | 414 | 4.82 | 4.5E-04 | 1.2E-02 | | 3.1E-01 |
| 197 | Trichlorobenzene, 1,2,4- | 120821 | 181.5 | 3.98 | 2.6E-03 | 6.6E-02 | | 1.7E+00 |
| ** 198 | Trichloroethane, 1,1,1- | 71556 | 133.4 | 2.49 | 5.1E-04 | 1.3E-02 | | 3.1E-01 |
| ** 199 | Trichloroethane, 1,1,2- | 79005 | 133.4 | 2.05 | 2.6E-04 | 6.4E-03 | | 1.6E-01 |
| ** 200 | Trichloroethylene | 79016 | 131.4 | 2.42 | 4.7E-04 | 1.2E-02 | | 2.9E-01 |
| ** 201 | Trichlorofluoromethane | 75694 | 137.4 | 2.53 | 5.1E-04 | 1.3E-02 | | 3.2E-01 |
| 202 | <i>2,4,6-Trichlorophenol</i> | 88062 | 197.4 | 3.69 | 1.9E-02 | 3.5E-02 | 5.9E-02 | 6.2E-02 |
| * 203 | Tris(2,3-dibromopropyl)phosphate | 126727 | 697.6 | 4.98 | 1.3E-05 | 3.9E-04 | | 1.1E-02 |
| 204 | Tris(aziridinyl)-para-benzoquinone | 68768 | 231.3 | -1.34 | 3.7E-07 | 1.0E-05 | | 2.8E-04 |
| * 205 | Urea | 57136 | 60 | -2.11 | 9.9E-07 | 2.9E-05 | | 8.3E-04 |
| ** 206 | Vinyl bromide | 593602 | 107 | 1.57 | 1.8E-04 | 4.3E-03 | | 1.1E-01 |

EXHIBIT B-2**PREDICTED K_p FOR ORGANIC CONTAMINANTS IN WATER (continued)**

| | CHEMICAL | CAS No. | MW | log K _{ow} | K _p 95% LCL | K _p (cm/hr) predicted | K _p (cm/hr) measured | K _p 95% UCL |
|--------|----------------|---------|-------|---------------------|------------------------------|--|---------------------------------------|---------------------------|
| ** 207 | Vinyl chloride | 75014 | 62.5 | 1.36 | 2.2E-04 | 5.6E-03 | | 1.4E-01 |
| * 208 | Water | 7732185 | 18.01 | -1.38 | 5.8E-05 | 1.5E-04 | 5.0E-04 | 3.9E-04 |
| 209 | Xylene, m- | 108383 | 106.2 | 3.20 | 2.1E-03 | 5.3E-02 | | 1.4E+00 |

EXHIBIT B-3

CALCULATION OF DERMAL ABSORBED DOSE FOR ORGANIC CHEMICALS IN WATER

Note: The following default exposure conditions are used to calculate exposure to chemicals in water through showering, assuming carcinogenic effects. Site-specific exposure conditions should be used in the spreadsheet ORG04_01.WK4 for appropriate health effects (cancer or noncancer).

Concentration in ppb (1 ppb = 1 µg/L x mg/1000 µg x L/1000 cm³):

Conc = 1 ppm = 1000 ppb = 1000 µg/L = 1 mg/L = 10⁻³ mg/cm³ (default value for purpose of illustration)

(site-specific concentration should be used in actual calculations)

Surface area exposed (cm²): SA = 18000 cm²

Event time (hr/event): t_{event} = 0.58 hr/event (35 minutes/event)

Event frequency (events/day): EV = 1.0 event/day

Exposure frequency (days/year): EF = 350.0 days/yr

Exposure duration (years): ED = 30.0 years

Body weight (kg): BW = 70.0 kg

Averaging time (days): AT = 25550 days

for carcinogenic effects, AT = 70 years (25550 days)

for noncarcinogenic effects, AT = ED (in days)

Skin thickness (assumed to be 10 µm): l_{sc} = 10⁻³ cm

Time to reach steady-state (hr): t* is chemical-specific

Fraction absorbed (FA, from Exhibit A-5, to the nearest one significant figure)

K_p used in the calculation of DA_{event} is the K_p predicted for all chemicals

Default conditions for screening purposes: Compare Dermal adults (showering for 35 minutes per day) to Oral adults (drinking 2 liters of water per day)

DAD (mg/day) = DA_{event} x SA x EV

Oral Dose (mg/day) = Conc x IR x ABS_{GI}

IR: Ingestion rate of drinking water = 2000 (cm³/day = L/day x 1000 cm³/L)

ABS_{GI}: Absorption fraction in GI tract = 1.0 (assuming 100% GI absorption)

The actual ratio Dermal/Oral is given in the column labeled “Derm/Oral”, the next column “Chem Assess” gives the result of the comparison of these two routes of exposure as “Y” when Dermal Exposure exceeds 10% of Drinking Water (ratio of DAD from Dermal to Oral). The Oral route is represented by drinking 2 liters of water per day.

The spreadsheet (ORG04_01.WK4) also provides the calculation of the ratio of the dermal dose absorbed to the total dose available from a showering scenario, assuming 5 gallons/minute as a flow rate. Refer to Chapter 3 and Appendix A for equations to evaluate DA_{event} and DAD.

All calculations are performed using the Lotus spreadsheet software, except otherwise noted.

For chemicals noted with “*” or “**”, see Notes on Exhibit B-2.

EXHIBIT B-3
**CALCULATION OF DERMAL ABSORBED DOSE FOR
ORGANIC CHEMICALS IN WATER (continued)**

| | CHEMICAL | CAS No. | K_p (cm/hr) | B | t (hr) | t* (hr) | FA | DA_{event} (mg/cm² -event) | DAD (mg/kg -day) | Derm/ Oral (%) | Chem Assess |
|-------|---------------------------------|----------------|----------------------------------|----------|-------------------|--------------------|-----------|--|---------------------------------|-------------------------------|------------------------|
| 1 | Acetaldehyde | 75070 | 6.3E-04 | 0.0 | 0.19 | 0.45 | 1.0 | 6.1E-07 | 6.4E-05 | 1% | N |
| 2 | Acetamide | 60355 | 1.1E-04 | 0.0 | 0.23 | 0.55 | 1.0 | 1.1E-07 | 1.2E-05 | 0% | N |
| 3 | Acetylaminofluorene, 2- | 53963 | 1.2E-02 | 0.1 | 1.90 | 4.56 | 1.0 | 3.6E-05 | 3.8E-03 | 33% | Y |
| 4 | Acrolein | 107028 | 6.5E-04 | 0.0 | 0.22 | 0.53 | 1.0 | 6.7E-07 | 7.0E-05 | 1% | N |
| 5 | Acrylamide | 79061 | 2.2E-04 | 0.0 | 0.27 | 0.64 | 1.0 | 2.4E-07 | 2.6E-05 | 0% | N |
| 6 | Acrylonitrile | 107131 | 1.2E-03 | 0.0 | 0.21 | 0.51 | 1.0 | 1.2E-06 | 1.2E-04 | 1% | N |
| 7 | Aldrin | 309002 | 1.4E-03 | 0.0 | 11.89 | 28.54 | 1.0 | 1.0E-05 | 1.1E-03 | 9% | N |
| ** 8 | Allyl chloride | 107051 | 5.4E-03 | 0.0 | 0.29 | 0.69 | 1.0 | 6.1E-06 | 6.4E-04 | 5% | N |
| 9 | Amino-2-methylanthraquinone, 1- | 82280 | 5.3E-03 | 0.0 | 2.28 | 5.48 | 1.0 | 1.7E-05 | 1.8E-03 | 15% | Y |
| 10 | Aminoanthraquinone, 2- | 117793 | 2.4E-03 | 0.0 | 1.90 | 4.56 | 1.0 | 6.9E-06 | 7.2E-04 | 6% | N |
| 11 | Aminoazobenzene, p- | 60093 | 6.8E-03 | 0.0 | 1.36 | 3.26 | 1.0 | 1.7E-05 | 1.8E-03 | 15% | Y |
| 12 | Aminoazotoluene, o- | 97563 | 3.4E-02 | 0.2 | 1.96 | 4.69 | 1.0 | 1.0E-04 | 1.1E-02 | 91% | Y |
| 13 | Aminobiphenyl, 4- | 92671 | 1.3E-02 | 0.1 | 0.95 | 2.27 | 1.0 | 2.6E-05 | 2.8E-03 | 24% | Y |
| 14 | Aniline | 62533 | 1.9E-03 | 0.0 | 0.35 | 0.85 | 1.0 | 2.3E-06 | 2.5E-04 | 2% | N |
| 15 | Anisidine, o- | 90040 | 1.5E-03 | 0.0 | 0.69 | 1.66 | 1.0 | 2.6E-06 | 2.7E-04 | 2% | N |
| 16 | Auramine | 492808 | 1.1E-02 | 0.1 | 3.37 | 8.09 | 0.9 | 3.9E-05 | 4.1E-03 | 35% | Y |
| 17 | Benzene | 71432 | 1.5E-02 | 0.1 | 0.29 | 0.70 | 1.0 | 1.7E-05 | 1.8E-03 | 15% | Y |
| 18 | Benzidine | 92875 | 1.1E-03 | 0.0 | 1.15 | 2.76 | 1.0 | 2.6E-06 | 2.7E-04 | 2% | N |
| * 19 | Benzo-a-anthracene | 56553 | 4.7E-01 | 2.8 | 2.03 | 8.53 | 1.0 | 1.4E-03 | 1.5E-01 | 1283% | Y |
| * 20 | Benzo-a-pyrene | 50328 | 7.0E-01 | 4.3 | 2.69 | 11.67 | 1.0 | 2.4E-03 | 2.6E-01 | 2186% | Y |
| * 21 | Benzo-b-fluoranthene | 205992 | 7.0E-01 | 4.3 | 2.77 | 12.03 | 1.0 | 2.5E-03 | 2.6E-01 | 2221% | Y |
| 22 | Benzoic acid | 65850 | 5.7E-03 | 0.0 | 0.51 | 1.24 | 1.0 | 8.6E-06 | 9.1E-04 | 8% | N |
| 23 | Benzotrichloride | 98077 | 1.1E-02 | 0.1 | 1.32 | 3.17 | 1.0 | 2.7E-05 | 2.8E-03 | 24% | Y |
| 24 | Benzyl chloride | 100447 | 1.0E-02 | 0.0 | 0.55 | 1.32 | 1.0 | 1.6E-05 | 1.7E-03 | 14% | Y |
| 25 | Bis(2-chloroethyl)ether | 111444 | 1.8E-03 | 0.0 | 0.68 | 1.62 | 1.0 | 3.1E-06 | 3.3E-04 | 3% | N |
| ** 26 | Bromodichloromethane | 75274 | 4.6E-03 | 0.0 | 0.88 | 2.12 | 1.0 | 9.2E-06 | 9.7E-04 | 8% | N |
| ** 27 | Bromoform | 75252 | 2.2E-03 | 0.0 | 2.79 | 6.70 | 1.0 | 7.9E-06 | 8.4E-04 | 7% | N |
| ** 28 | Bromomethane | 74839 | 2.8E-03 | 0.0 | 0.36 | 0.87 | 1.0 | 3.6E-06 | 3.8E-04 | 3% | N |
| 29 | Bromophenol, p- | 106412 | 8.8E-03 | 0.0 | 0.99 | 2.39 | 1.0 | 1.9E-05 | 2.0E-03 | 17% | Y |
| 30 | Butadiene, 1,3- | 106990 | 1.6E-02 | 0.0 | 0.21 | 0.51 | 1.0 | 1.6E-05 | 1.7E-03 | 15% | Y |
| 31 | 2,3-Butanediol | 513859 | 1.2E-04 | 0.0 | 0.34 | 0.82 | 1.0 | 1.5E-07 | 1.6E-05 | 0% | N |
| 32 | n-Butanol | 71363 | 2.3E-03 | 0.0 | 0.28 | 0.67 | 1.0 | 2.6E-06 | 2.7E-04 | 2% | N |
| 33 | Butoxyethanol, 2- | 111762 | 1.2E-03 | 0.0 | 0.49 | 1.17 | 1.0 | 1.8E-06 | 1.9E-04 | 2% | N |
| 34 | Captan | 133062 | 1.2E-03 | 0.0 | 5.13 | 12.32 | 1.0 | 5.7E-06 | 6.0E-04 | 5% | N |
| 35 | Carbon disulfide | 75150 | 1.7E-02 | 0.1 | 0.30 | 0.72 | 1.0 | 2.0E-05 | 2.1E-03 | 18% | Y |

EXHIBIT B-3
**CALCULATION OF DERMAL ABSORBED DOSE FOR
ORGANIC CHEMICALS IN WATER (continued)**

| | CHEMICAL | CAS No. | K _p (cm/hr) | B | t (hr) | t* (hr) | FA | DA _{event} (mg/cm ² -event) | DAD (mg/kg -day) | Derm/ Oral (%) | Chem Assess |
|-------|---------------------------|---------|---------------------------|-----|-----------|------------|-----|---|------------------------|----------------------|----------------|
| ** 36 | Carbon tetrachloride | 56235 | 1.6E-02 | 0.1 | 0.78 | 1.86 | 1.0 | 3.0E-05 | 3.2E-03 | 27% | Y |
| 37 | Chlordane | 57749 | 3.8E-02 | 0.3 | 21.21 | 50.91 | 0.7 | 2.6E-04 | 2.7E-02 | 231% | Y |
| 38 | Chlordane (cis) | 5103719 | 3.4E-02 | 0.3 | 21.27 | 51.05 | 0.7 | 2.3E-04 | 2.4E-02 | 208% | Y |
| 39 | Chlordane (trans) | 5103742 | 3.4E-02 | 0.3 | 21.27 | 51.05 | 0.7 | 2.3E-04 | 2.4E-02 | 208% | Y |
| 40 | Chlorobenzene | 108907 | 2.8E-02 | 0.1 | 0.46 | 1.09 | 1.0 | 4.0E-05 | 4.2E-03 | 36% | Y |
| 41 | 4-Chlorocresol | 59507 | 2.9E-02 | 0.1 | 0.67 | 1.61 | 1.0 | 4.9E-05 | 5.2E-03 | 44% | Y |
| ** 42 | Chlorodibromomethane | 124481 | 3.2E-03 | 0.0 | 1.57 | 3.77 | 1.0 | 8.5E-06 | 9.0E-04 | 8% | N |
| ** 43 | Chloroethane | 75003 | 6.1E-03 | 0.0 | 0.24 | 0.59 | 1.0 | 6.3E-06 | 6.7E-04 | 6% | N |
| ** 44 | Chloroform | 67663 | 6.8E-03 | 0.0 | 0.50 | 1.19 | 1.0 | 1.0E-05 | 1.1E-03 | 9% | N |
| ** 45 | Chloromethane | 74873 | 3.3E-03 | 0.0 | 0.20 | 0.49 | 1.0 | 3.3E-06 | 3.4E-04 | 3% | N |
| 46 | 2-Chlorophenol | 95578 | 8.0E-03 | 0.0 | 0.56 | 1.34 | 1.0 | 1.3E-05 | 1.3E-03 | 11% | Y |
| 47 | 4-Chlorophenol | 106489 | 1.2E-02 | 0.1 | 0.56 | 1.34 | 1.0 | 1.8E-05 | 1.9E-03 | 16% | Y |
| 48 | Chlorothalonil | 1897456 | 1.9E-02 | 0.1 | 3.30 | 7.93 | 0.9 | 6.4E-05 | 6.8E-03 | 58% | Y |
| * 49 | Chrysene | 218019 | 4.7E-01 | 2.8 | 2.03 | 8.53 | 1.0 | 1.4E-03 | 1.5E-01 | 1283% | Y |
| 50 | Cresidine, p- | 120718 | 3.4E-03 | 0.0 | 0.63 | 1.50 | 1.0 | 5.7E-06 | 6.0E-04 | 5% | N |
| 51 | m-Cresol | 108394 | 7.8E-03 | 0.0 | 0.43 | 1.03 | 1.0 | 1.1E-05 | 1.1E-03 | 10% | N |
| 52 | o-Cresol | 95487 | 7.7E-03 | 0.0 | 0.43 | 1.03 | 1.0 | 1.1E-05 | 1.1E-03 | 10% | N |
| 53 | p-Cresol | 106445 | 7.7E-03 | 0.0 | 0.43 | 1.03 | 1.0 | 1.1E-05 | 1.1E-03 | 10% | N |
| * 54 | DDD | 72548 | 1.8E-01 | 1.2 | 6.65 | 25.99 | 0.8 | 7.8E-04 | 8.3E-02 | 703% | Y |
| * 55 | DDE | 72559 | 1.6E-01 | 1.1 | 6.48 | 25.08 | 0.8 | 6.7E-04 | 7.1E-02 | 602% | Y |
| * 56 | DDT | 50293 | 2.7E-01 | 1.9 | 10.45 | 42.51 | 0.7 | 1.3E-03 | 1.4E-01 | 1156% | Y |
| * 57 | n-Decanol | 112301 | 2.2E-01 | 1.1 | 0.82 | 3.18 | 1.0 | 4.2E-04 | 4.5E-02 | 380% | Y |
| 58 | Di-2-ethylhexyl phthalate | 117817 | 2.5E-02 | 0.2 | 16.64 | 39.93 | 0.8 | 1.7E-04 | 1.8E-02 | 155% | Y |
| 59 | Diaminoanisole, 2,4- | 615054 | 2.2E-04 | 0.0 | 0.63 | 1.52 | 1.0 | 3.7E-07 | 3.9E-05 | 0% | N |
| 60 | Diaminotoluene | 95807 | 5.4E-04 | 0.0 | 0.51 | 1.24 | 1.0 | 8.3E-07 | 8.7E-05 | 1% | N |
| 61 | Diaminotoluene, 2,4- | 101804 | 2.8E-03 | 0.0 | 1.41 | 3.38 | 1.0 | 6.9E-06 | 7.3E-04 | 6% | N |
| * 62 | Dibenzo(a,h)anthracene | 53703 | 1.5E+00 | 9.7 | 3.88 | 17.57 | 0.6 | 3.8E-03 | 4.0E-01 | 3388% | Y |
| 63 | Dibutyl phthalate | 84742 | 2.4E-02 | 0.2 | 3.86 | 9.27 | 0.9 | 9.0E-05 | 9.5E-03 | 81% | Y |
| 64 | Dichlorobenzene, 1,2- | 95501 | 4.1E-02 | 0.2 | 0.71 | 1.71 | 1.0 | 7.4E-05 | 7.8E-03 | 66% | Y |
| 65 | Dichlorobenzene, 1,3- | 541731 | 5.8E-02 | 0.3 | 0.71 | 1.71 | 1.0 | 1.0E-04 | 1.1E-02 | 93% | Y |
| 66 | Dichlorobenzene, 1,4- | 106467 | 4.2E-02 | 0.2 | 0.71 | 1.71 | 1.0 | 7.5E-05 | 7.9E-03 | 67% | Y |
| 67 | Dichlorobenzidine, 3,3' | 91941 | 1.3E-02 | 0.1 | 2.80 | 6.72 | 1.0 | 4.5E-05 | 4.8E-03 | 41% | Y |
| ** 68 | Dichlorodifluoromethane | 75718 | 9.0E-03 | 0.0 | 0.51 | 1.22 | 1.0 | 1.3E-05 | 1.4E-03 | 12% | Y |
| ** 69 | Dichloroethane, 1,1- | 75343 | 6.7E-03 | 0.0 | 0.38 | 0.92 | 1.0 | 8.8E-06 | 9.3E-04 | 8% | N |
| ** 70 | Dichloroethane, 1,2- | 107062 | 4.2E-03 | 0.0 | 0.38 | 0.92 | 1.0 | 5.5E-06 | 5.8E-04 | 5% | N |
| ** 71 | Dichloroethylene, 1,1- | 75354 | 1.2E-02 | 0.0 | 0.37 | 0.89 | 1.0 | 1.5E-05 | 1.6E-03 | 14% | Y |

EXHIBIT B-3
**CALCULATION OF DERMAL ABSORBED DOSE FOR
ORGANIC CHEMICALS IN WATER (continued)**

| | CHEMICAL | CAS No. | K_p (cm/hr) | B | t (hr) | t* (hr) | FA | DA_{event} (mg/cm² -event) | DAD (mg/kg -day) | Derm/ Oral (%) | Chem Assess |
|-------|-------------------------------|----------------|----------------------------------|----------|-------------------|--------------------|-----------|--|---------------------------------|-------------------------------|------------------------|
| ** 72 | Dichloroethylene, 1,2-(trans) | 540590 | 7.7E-03 | 0.0 | 0.37 | 0.89 | 1.0 | 9.9E-06 | 1.0E-03 | 9% | N |
| 73 | 2,4-Dichlorophenol | 120832 | 2.1E-02 | 0.1 | 0.87 | 2.10 | 1.0 | 4.1E-05 | 4.3E-03 | 37% | Y |
| ** 74 | Dichloropropane, 1,2- | 78875 | 7.8E-03 | 0.0 | 0.46 | 1.10 | 1.0 | 1.1E-05 | 1.2E-03 | 10% | N |
| ** 75 | Dichloropropene, 1,3- | 542756 | 4.3E-03 | 0.0 | 0.45 | 1.07 | 1.0 | 6.1E-06 | 6.4E-04 | 5% | N |
| 76 | Dichlorvos | 62737 | 8.5E-04 | 0.0 | 1.85 | 4.44 | 1.0 | 2.5E-06 | 2.6E-04 | 2% | N |
| 77 | Dieldrin | 60571 | 1.2E-02 | 0.1 | 14.62 | 35.09 | 0.8 | 7.9E-05 | 8.3E-03 | 71% | Y |
| 78 | Diepoxybutane | 1464535 | 3.1E-05 | 0.0 | 0.32 | 0.78 | 1.0 | 3.7E-08 | 3.9E-06 | 0% | N |
| 79 | Diethyl phthalate | 84662 | 3.9E-03 | 0.0 | 1.87 | 4.50 | 1.0 | 1.1E-05 | 1.2E-03 | 10% | Y |
| 80 | Diethyl sulfate | 64675 | 1.2E-03 | 0.0 | 0.78 | 1.87 | 1.0 | 2.3E-06 | 2.4E-04 | 2% | N |
| 81 | Dimethoxybenzidine, 3,3'- | 119904 | 9.3E-04 | 0.0 | 2.85 | 6.84 | 1.0 | 3.3E-06 | 3.5E-04 | 3% | N |
| 82 | Dimethyl phthalate | 131113 | 1.4E-03 | 0.0 | 1.30 | 3.13 | 1.0 | 3.4E-06 | 3.5E-04 | 3% | N |
| 83 | Dimethyl sulfate | 77781 | 1.8E-03 | 0.0 | 0.54 | 1.30 | 1.0 | 2.8E-06 | 3.0E-04 | 3% | N |
| 84 | Dimethylamine, n-nitroso- | 62759 | 2.5E-04 | 0.0 | 0.28 | 0.67 | 1.0 | 2.8E-07 | 3.0E-05 | 0% | N |
| 85 | Dimethylaminoazobenzene, 4- | 60117 | 9.5E-02 | 0.5 | 1.95 | 4.67 | 1.0 | 2.8E-04 | 2.9E-02 | 251% | Y |
| 86 | Dimethylbenzidine, 3,3'- | 119937 | 3.6E-03 | 0.0 | 1.65 | 3.97 | 1.0 | 9.8E-06 | 1.0E-03 | 9% | N |
| 87 | Dimethylcarbamyl chloride | 79447 | 3.9E-04 | 0.0 | 0.43 | 1.02 | 1.0 | 5.4E-07 | 5.7E-05 | 0% | N |
| 88 | Dimethylhydrazine, 1,1- | 57147 | 7.3E-05 | 0.0 | 0.23 | 0.55 | 1.0 | 7.6E-08 | 8.0E-06 | 0% | N |
| 89 | Dimethylphenol, 2,4- | 105679 | 1.1E-02 | 0.0 | 0.52 | 1.24 | 1.0 | 1.7E-05 | 1.7E-03 | 15% | Y |
| 90 | Dimethylphenol, 3,4- | 95658 | 9.8E-03 | 0.0 | 0.51 | 1.24 | 1.0 | 1.5E-05 | 1.6E-03 | 13% | Y |
| 91 | Dinitrophenol, 2,4- | 51285 | 1.5E-03 | 0.0 | 1.15 | 2.76 | 1.0 | 3.5E-06 | 3.7E-04 | 3% | N |
| 92 | Dinitrotoluene, 2,4- | 121142 | 3.1E-03 | 0.0 | 1.12 | 2.69 | 1.0 | 6.9E-06 | 7.3E-04 | 6% | N |
| 93 | Dinitrotoluene, 2,6- | 606202 | 2.1E-03 | 0.0 | 1.12 | 2.69 | 1.0 | 4.6E-06 | 4.9E-04 | 4% | N |
| 94 | Dioxane, 1,4- | 123911 | 3.3E-04 | 0.0 | 0.33 | 0.80 | 1.0 | 4.0E-07 | 4.3E-05 | 0% | N |
| 95 | Diphenylamine, n-nitroso- | 86306 | 1.5E-02 | 0.1 | 1.38 | 3.31 | 1.0 | 3.6E-05 | 3.8E-03 | 32% | Y |
| 96 | Diphenylhydrazine, 1,2- | 122667 | 1.3E-02 | 0.1 | 1.15 | 2.76 | 1.0 | 3.0E-05 | 3.1E-03 | 27% | Y |
| 97 | Dipropylamine, n-nitroso- | 621647 | 2.3E-03 | 0.0 | 0.57 | 1.37 | 1.0 | 3.7E-06 | 3.9E-04 | 3% | N |
| 98 | Endrin | 72208 | 1.2E-02 | 0.1 | 14.62 | 35.09 | 0.8 | 7.9E-05 | 8.3E-03 | 71% | Y |
| 99 | Epichlorohydrin | 106898 | 3.5E-04 | 0.0 | 0.35 | 0.84 | 1.0 | 4.3E-07 | 4.6E-05 | 0% | N |
| 100 | Ethanol | 64175 | 5.4E-04 | 0.0 | 0.19 | 0.46 | 1.0 | 5.2E-07 | 5.5E-05 | 0% | N |
| 101 | Ethanol, 2-(2-butoxyethoxy)- | 112345 | 4.7E-05 | 0.0 | 0.86 | 2.07 | 1.0 | 9.3E-08 | 9.8E-06 | 0% | N |
| 102 | Ethanol, 2-(2-ethoxyethoxy)- | 111900 | 2.5E-04 | 0.0 | 0.60 | 1.44 | 1.0 | 4.0E-07 | 4.2E-05 | 0% | N |

EXHIBIT B-3
**CALCULATION OF DERMAL ABSORBED DOSE FOR
ORGANIC CHEMICALS IN WATER (continued)**

| | CHEMICAL | CAS No. | K_p (cm/hr) | B | t (hr) | t* (hr) | FA | DA_{event} (mg/cm² -event) | DAD (mg/kg -day) | Derm/ Oral (%) | Chem Assess |
|--------|----------------------------------|----------------|----------------------------------|----------|-------------------|--------------------|-----------|--|---------------------------------|-------------------------------|------------------------|
| 103 | Ethanol, 2-(2-methoxyethoxy)- | 111773 | 1.7E-04 | 0.0 | 0.50 | 1.20 | 1.0 | 2.6E-07 | 2.8E-05 | 0% | N |
| 104 | 2-Ethoxy ethanol (Cellosolve) | 110805 | 3.0E-04 | 0.0 | 0.34 | 0.82 | 1.0 | 3.7E-07 | 3.9E-05 | 0% | N |
| 105 | Ethoxyethyl acetate, 2- | 111159 | 7.7E-04 | 0.0 | 0.59 | 1.41 | 1.0 | 1.2E-06 | 1.3E-04 | 1% | N |
| 106 | Ethyl acrylate | 140885 | 3.2E-03 | 0.0 | 0.39 | 0.93 | 1.0 | 4.3E-06 | 4.5E-04 | 4% | N |
| 107 | Ethyl carbamate | 51796 | 3.9E-04 | 0.0 | 0.34 | 0.81 | 1.0 | 4.8E-07 | 5.1E-05 | 0% | N |
| 108 | Ethyl ether | 60297 | 2.3E-03 | 0.0 | 0.28 | 0.67 | 1.0 | 2.6E-06 | 2.8E-04 | 2% | N |
| 109 | Ethylbenzene | 100414 | 4.9E-02 | 0.2 | 0.42 | 1.01 | 1.0 | 6.7E-05 | 7.1E-03 | 61% | Y |
| 110 | Ethylene oxide | 75218 | 5.6E-04 | 0.0 | 0.19 | 0.45 | 1.0 | 5.4E-07 | 5.7E-05 | 0% | N |
| ** 111 | Ethylenedibromide | 106934 | 2.8E-03 | 0.0 | 1.21 | 2.90 | 1.0 | 6.4E-06 | 6.8E-04 | 6% | N |
| 112 | Ethyleneimine | 151564 | 1.6E-04 | 0.0 | 0.19 | 0.45 | 1.0 | 1.5E-07 | 1.6E-05 | 0% | N |
| 113 | Ethylenethiourea | 96457 | 1.7E-04 | 0.0 | 0.37 | 0.88 | 1.0 | 2.1E-07 | 2.2E-05 | 0% | N |
| 114 | 4-Ethylphenol | 123079 | 1.7E-02 | 0.1 | 0.52 | 1.24 | 1.0 | 2.5E-05 | 2.7E-03 | 23% | Y |
| * 115 | Fluoranthene | 206440 | 2.2E-01 | 1.2 | 1.45 | 5.68 | 1.0 | 5.7E-04 | 6.0E-02 | 512% | Y |
| 116 | Formaldehyde | 50000 | 1.8E-03 | 0.0 | 0.16 | 0.38 | 1.0 | 1.6E-06 | 1.7E-04 | 1% | N |
| 117 | Glycerol | 56815 | 3.2E-05 | 0.0 | 0.35 | 0.84 | 1.0 | 4.0E-08 | 4.3E-06 | 0% | N |
| 118 | Heptachlor | 76448 | 8.6E-03 | 0.1 | 13.27 | 31.85 | 0.8 | 5.3E-05 | 5.6E-03 | 48% | Y |
| 119 | n-Heptanol | 111706 | 1.9E-02 | 0.1 | 0.48 | 1.15 | 1.0 | 2.8E-05 | 3.0E-03 | 25% | Y |
| * 120 | Hexachlorobenzene | 118741 | 1.3E-01 | 0.9 | 4.22 | 16.21 | 0.9 | 5.2E-04 | 5.5E-02 | 469% | Y |
| ** 121 | Hexachlorobutadiene | 87683 | 8.1E-02 | 0.5 | 3.09 | 7.42 | 0.9 | 2.7E-04 | 2.9E-02 | 243% | Y |
| ** 122 | Hexachloroethane | 67721 | 3.0E-02 | 0.2 | 2.27 | 5.44 | 1.0 | 9.6E-05 | 1.0E-02 | 86% | Y |
| 123 | Hexamethylphosphoramide | 680319 | 1.6E-04 | 0.0 | 1.08 | 2.58 | 1.0 | 3.6E-07 | 3.8E-05 | 0% | N |
| 124 | n-Hexanol | 111273 | 9.3E-03 | 0.0 | 0.40 | 0.96 | 1.0 | 1.2E-05 | 1.3E-03 | 11% | Y |
| * 125 | Hydrazine/Hydrazine sulfate | 302012 | 4.4E-05 | 0.0 | 0.16 | 0.39 | 1.0 | 3.9E-08 | 4.2E-06 | 0% | N |
| * 126 | Indeno(1,2,3-CD)pyrene | 193395 | 1.0E+00 | 6.7 | 3.78 | 16.83 | 0.6 | 2.6E-03 | 2.7E-01 | 2307% | Y |
| 127 | Isophorone | 78591 | 3.4E-03 | 0.0 | 0.63 | 1.52 | 1.0 | 5.7E-06 | 6.0E-04 | 5% | N |
| 128 | Lindane | 58899 | 1.1E-02 | 0.1 | 4.57 | 10.97 | 0.9 | 4.4E-05 | 4.6E-03 | 40% | Y |
| 129 | Mechlorethamine | 51752 | 1.1E-03 | 0.0 | 0.80 | 1.92 | 1.0 | 2.0E-06 | 2.1E-04 | 2% | N |
| 130 | Methanol | 67561 | 3.2E-04 | 0.0 | 0.16 | 0.39 | 1.0 | 2.9E-07 | 3.0E-05 | 0% | N |
| 131 | Methoxyethanol, 2- | 109864 | 1.8E-04 | 0.0 | 0.28 | 0.68 | 1.0 | 2.0E-07 | 2.1E-05 | 0% | N |
| 132 | Methoxypalan-2-ol, 1- | 107982 | 3.7E-04 | 0.0 | 0.34 | 0.82 | 1.0 | 4.6E-07 | 4.8E-05 | 0% | N |
| 133 | Methyl ethyl ketone | 78933 | 9.6E-04 | 0.0 | 0.27 | 0.65 | 1.0 | 1.1E-06 | 1.1E-04 | 1% | N |
| 134 | Methyl-4-hydroxy benzoate | 99763 | 4.4E-03 | 0.0 | 0.76 | 1.82 | 1.0 | 8.1E-06 | 8.6E-04 | 7% | N |
| ** 135 | Methyl iodide | 74884 | 2.5E-03 | 0.0 | 0.67 | 1.60 | 1.0 | 4.3E-06 | 4.6E-04 | 4% | N |
| 136 | Methylaziridine, 2- | 75558 | 3.0E-04 | 0.0 | 0.22 | 0.53 | 1.0 | 3.1E-07 | 3.3E-05 | 0% | N |

EXHIBIT B-3**CALCULATION OF DERMAL ABSORBED DOSE FOR
ORGANIC CHEMICALS IN WATER (continued)**

| | CHEMICAL | CAS No. | K_p (cm/hr) | B | t (hr) | t* (hr) | FA | DA_{event} (mg/cm² -event) | DAD (mg/kg -day) | Derm/ Oral (%) | Chem Assess |
|--------|---|----------------|----------------------------------|----------|-------------------|--------------------|-----------|--|---------------------------------|-------------------------------|------------------------|
| 137 | Methylene bis(2-chloroaniline), 4,4'- | 101144 | 2.1E-02 | 0.1 | 3.36 | 8.06 | 0.9 | 7.2E-05 | 7.6E-03 | 65% | Y |
| 138 | Methylene bis(N,N'-dimethyl)aniline , 4,4'- | 101611 | 8.4E-02 | 0.5 | 2.83 | 6.80 | 1.0 | 3.0E-04 | 3.2E-02 | 270% | Y |
| ** 139 | Methylene chloride | 75092 | 3.5E-03 | 0.0 | 0.32 | 0.76 | 1.0 | 4.2E-06 | 4.5E-04 | 4% | N |
| 140 | Methylenedianiline, 4,4'- | 101779 | 1.4E-03 | 0.0 | 1.37 | 3.30 | 1.0 | 3.4E-06 | 3.6E-04 | 3% | N |
| 141 | Michler's ketone | 90948 | 2.5E-02 | 0.2 | 3.41 | 8.19 | 0.9 | 8.7E-05 | 9.2E-03 | 78% | Y |
| ** 142 | Mustard Gas | 505602 | 4.5E-03 | 0.0 | 0.83 | 2.00 | 1.0 | 8.6E-06 | 9.1E-04 | 8% | N |
| 143 | Naphthalene | 91203 | 4.7E-02 | 0.2 | 0.56 | 1.34 | 1.0 | 7.4E-05 | 7.8E-03 | 66% | Y |
| 144 | 2-Naphthol | 135193 | 1.9E-02 | 0.1 | 0.69 | 1.64 | 1.0 | 3.3E-05 | 3.5E-03 | 30% | Y |
| 145 | Naphthylamine, 1- | 134327 | 7.7E-03 | 0.0 | 0.68 | 1.62 | 1.0 | 1.3E-05 | 1.4E-03 | 12% | Y |
| 146 | Naphthylamine, 2- | 91598 | 8.1E-03 | 0.0 | 0.68 | 1.62 | 1.0 | 1.4E-05 | 1.5E-03 | 13% | Y |
| 147 | Nitrolotriacetic acid | 139139 | 1.0E-04 | 0.0 | 1.26 | 3.01 | 1.0 | 2.4E-07 | 2.5E-05 | 0% | N |
| 148 | Nitro-o-anisidine, 5- | 99592 | 2.1E-03 | 0.0 | 0.77 | 1.84 | 1.0 | 3.8E-06 | 4.0E-04 | 3% | N |
| 149 | Nitrobiphenyl, 4- | 92933 | 3.8E-02 | 0.2 | 1.40 | 3.35 | 1.0 | 9.5E-05 | 1.0E-02 | 86% | Y |
| * 150 | Nitrofen | 1836755 | 1.9E-01 | 1.2 | 4.18 | 16.33 | 0.9 | 7.3E-04 | 7.7E-02 | 660% | Y |
| 151 | Nitrophenol, 2- | 88755 | 4.0E-03 | 0.0 | 0.64 | 1.54 | 1.0 | 6.8E-06 | 7.2E-04 | 6% | N |
| 152 | Nitrophenol, 2-amino-4- | 99570 | 1.7E-03 | 0.0 | 0.78 | 1.87 | 1.0 | 3.2E-06 | 3.4E-04 | 3% | N |
| 153 | 3-Nitrophenol | 554847 | 5.5E-03 | 0.0 | 0.64 | 1.54 | 1.0 | 9.4E-06 | 9.9E-04 | 8% | N |
| 154 | 4-Nitrophenol | 100027 | 4.8E-03 | 0.0 | 0.64 | 1.54 | 1.0 | 8.2E-06 | 8.6E-04 | 7% | N |
| 155 | Nitrophenol, 4-amino-2- | 119346 | 9.3E-04 | 0.0 | 0.78 | 1.87 | 1.0 | 1.7E-06 | 1.8E-04 | 2% | N |
| 156 | Nitropropane, 2- | 79469 | 8.8E-04 | 0.0 | 0.44 | 1.06 | 1.0 | 1.2E-06 | 1.3E-04 | 1% | N |
| 157 | Nitroso-di-n-butylamine, n- | 924163 | 3.8E-03 | 0.0 | 0.82 | 1.97 | 1.0 | 7.3E-06 | 7.7E-04 | 7% | N |
| 158 | Nitroso-N-ethylurea, n- | 759739 | 4.9E-04 | 0.0 | 0.48 | 1.16 | 1.0 | 7.2E-07 | 7.6E-05 | 1% | N |
| 159 | Nitroso-N-methylurea, n- | 684935 | 3.9E-04 | 0.0 | 0.40 | 0.97 | 1.0 | 5.3E-07 | 5.6E-05 | 0% | N |
| 160 | Nitrosodietanolamine, n- | 1116547 | 2.5E-05 | 0.0 | 0.60 | 1.44 | 1.0 | 4.0E-08 | 4.3E-06 | 0% | N |
| 161 | Nitrosodiethylamine, n- | 55185 | 1.0E-03 | 0.0 | 0.33 | 0.80 | 1.0 | 1.3E-06 | 1.3E-04 | 1% | N |
| 162 | Nitrosodiphenylamine, p- | 156105 | 2.6E-02 | 0.1 | 1.38 | 3.31 | 1.0 | 6.4E-05 | 6.7E-03 | 57% | Y |
| 163 | Nitrosomethylvinylamine, n- | 4549400 | 5.1E-04 | 0.0 | 0.32 | 0.78 | 1.0 | 6.2E-07 | 6.5E-05 | 1% | N |
| 164 | Nitrosomorpholine, n- | 59892 | 1.8E-04 | 0.0 | 0.48 | 1.14 | 1.0 | 2.6E-07 | 2.7E-05 | 0% | N |
| 165 | Nitrosonornicotine, n- | 16543558 | 1.7E-04 | 0.0 | 1.05 | 2.52 | 1.0 | 3.6E-07 | 3.8E-05 | 0% | N |
| 166 | Nitrosopiperidine, n- | 100754 | 2.9E-05 | 0.0 | 9.83 | 23.60 | 1.0 | 1.9E-07 | 2.1E-05 | 0% | N |
| 167 | n-Nonanol | 143088 | 7.8E-02 | 0.4 | 0.69 | 1.65 | 1.0 | 1.4E-04 | 1.4E-02 | 122% | Y |

EXHIBIT B-3**CALCULATION OF DERMAL ABSORBED DOSE FOR
ORGANIC CHEMICALS IN WATER (continued)**

| | CHEMICAL | CAS No. | K _p (cm/hr) | B | t (hr) | t* (hr) | FA | DA _{event} (mg/cm ² -event) | DAD (mg/kg -day) | Derm/ Oral (%) | Chem Assess |
|--------|----------------------------------|----------|---------------------------|-----|-----------|------------|-----|---|------------------------|----------------------|----------------|
| 168 | n-Octanol | 111875 | 2.7E-02 | 0.1 | 0.57 | 1.37 | 1.0 | 4.4E-05 | 4.6E-03 | 39% | Y |
| 169 | Parathion | 56382 | 1.3E-02 | 0.1 | 4.57 | 10.97 | 0.9 | 5.2E-05 | 5.5E-03 | 47% | Y |
| * 170 | PCB-chlorobiphenyl, 4- | 2051629 | 7.5E-01 | 4.9 | 4.63 | 20.27 | 0.6 | 2.0E-03 | 2.2E-01 | 1844% | Y |
| * 171 | PCB-hexachlorobiphenyl | 26601649 | 4.3E-01 | 3.2 | 11.29 | 47.90 | 0.5 | 1.5E-03 | 1.6E-01 | 1378% | Y |
| ** 172 | Pentachloronitrobenzene | 82688 | 4.2E-02 | 0.3 | 4.83 | 11.60 | 0.9 | 1.7E-04 | 1.8E-02 | 157% | Y |
| * 173 | Pentachlorophenol | 87865 | 3.9E-01 | 2.5 | 3.33 | 13.82 | 0.9 | 1.4E-03 | 1.4E-01 | 1226% | Y |
| 174 | n-Pentanol | 71410 | 5.5E-03 | 0.0 | 0.33 | 0.80 | 1.0 | 6.6E-06 | 7.0E-04 | 6% | N |
| 175 | Pentanone, 4-methyl-2- | 108101 | 2.7E-03 | 0.0 | 0.39 | 0.93 | 1.0 | 3.5E-06 | 3.7E-04 | 3% | N |
| * 176 | Phenanthrene | 85018 | 1.4E-01 | 0.7 | 1.06 | 4.11 | 1.0 | 3.1E-04 | 3.3E-02 | 283% | Y |
| 177 | Phenol | 108952 | 4.3E-03 | 0.0 | 0.36 | 0.86 | 1.0 | 5.5E-06 | 5.8E-04 | 5% | N |
| 178 | Phenol, 4,6-dinitro-2-methyl- | 534521 | 3.1E-03 | 0.0 | 1.38 | 3.30 | 1.0 | 7.7E-06 | 8.1E-04 | 7% | N |
| 179 | n-Propanol | 71238 | 1.1E-03 | 0.0 | 0.23 | 0.56 | 1.0 | 1.1E-06 | 1.2E-04 | 1% | N |
| 180 | Propiolactone, beta- | 57578 | 3.1E-04 | 0.0 | 0.27 | 0.65 | 1.0 | 3.4E-07 | 3.5E-05 | 0% | N |
| 181 | Propylene oxide | 75569 | 7.7E-04 | 0.0 | 0.23 | 0.54 | 1.0 | 8.0E-07 | 8.5E-05 | 1% | N |
| 182 | Resorcinol | 108463 | 1.3E-03 | 0.0 | 0.44 | 1.06 | 1.0 | 1.8E-06 | 1.9E-04 | 2% | N |
| 183 | Safrole | 94597 | 1.1E-02 | 0.1 | 0.87 | 2.08 | 1.0 | 2.2E-05 | 2.3E-03 | 20% | Y |
| 184 | Styrene | 100425 | 3.7E-02 | 0.1 | 0.41 | 0.98 | 1.0 | 5.0E-05 | 5.3E-03 | 45% | Y |
| 185 | Styrene oxide | 96093 | 3.9E-03 | 0.0 | 0.50 | 1.20 | 1.0 | 5.8E-06 | 6.2E-04 | 5% | N |
| * 186 | TCDD | 1746016 | 8.1E-01 | 5.6 | 6.82 | 30.09 | 0.5 | 2.2E-03 | 2.4E-01 | 2003% | Y |
| ** 187 | Tetrachlorethylene | 127184 | 3.3E-02 | 0.2 | 0.91 | 2.18 | 1.0 | 6.7E-05 | 7.1E-03 | 60% | Y |
| ** 188 | Tetrachloroethane, 1,1,2,2- | 79345 | 6.9E-03 | 0.0 | 0.93 | 2.24 | 1.0 | 1.4E-05 | 1.5E-03 | 13% | Y |
| 189 | Thioacetamide | 62555 | 1.8E-03 | 0.0 | 0.28 | 0.67 | 1.0 | 2.0E-06 | 2.1E-04 | 2% | N |
| 190 | Thiodianiline, 4,4'- | 139651 | 2.1E-03 | 0.0 | 1.73 | 4.16 | 1.0 | 6.0E-06 | 6.3E-04 | 5% | N |
| 191 | Thiourea | 62566 | 1.4E-04 | 0.0 | 0.28 | 0.68 | 1.0 | 1.5E-07 | 1.6E-05 | 0% | N |
| 192 | Thymol | 89838 | 3.7E-02 | 0.2 | 0.74 | 1.78 | 1.0 | 6.8E-05 | 7.2E-03 | 61% | Y |
| 193 | Toluene | 108883 | 3.1E-02 | 0.1 | 0.35 | 0.84 | 1.0 | 3.9E-05 | 4.1E-03 | 35% | Y |
| 194 | Toluidine hydrochloride, o- | 636215 | 1.8E-03 | 0.0 | 0.68 | 1.62 | 1.0 | 3.1E-06 | 3.3E-04 | 3% | N |
| 195 | Toluidine, o- | 95534 | 3.0E-03 | 0.0 | 0.42 | 1.02 | 1.0 | 4.1E-06 | 4.3E-04 | 4% | N |
| 196 | Toxaphene | 8001352 | 1.2E-02 | 0.1 | 22.40 | 53.75 | 0.8 | 9.5E-05 | 1.0E-02 | 85% | Y |
| 197 | Trichlorobenzene, 1,2,4- | 120821 | 6.6E-02 | 0.3 | 1.11 | 2.66 | 1.0 | 1.5E-04 | 1.6E-02 | 133% | Y |
| ** 198 | Trichloroethane, 1,1,1- | 71556 | 1.3E-02 | 0.1 | 0.60 | 1.43 | 1.0 | 2.1E-05 | 2.2E-03 | 19% | Y |
| ** 199 | Trichloroethane, 1,1,2- | 79005 | 6.4E-03 | 0.0 | 0.60 | 1.43 | 1.0 | 1.0E-05 | 1.1E-03 | 9% | N |
| ** 200 | Trichloroethylene | 79016 | 1.2E-02 | 0.1 | 0.58 | 1.39 | 1.0 | 1.9E-05 | 2.0E-03 | 17% | Y |
| ** 201 | Trichlorofluoromethane | 75694 | 1.3E-02 | 0.1 | 0.63 | 1.51 | 1.0 | 2.1E-05 | 2.3E-03 | 19% | Y |

EXHIBIT B-3
**CALCULATION OF DERMAL ABSORBED DOSE FOR
ORGANIC CHEMICALS IN WATER (continued)**

| | CHEMICAL | CAS No. | K _p (cm/hr) | B | t (hr) | t* (hr) | FA | DA _{event} (mg/cm ² -event) | DAD (mg/kg -day) | Derm/ Oral (%) | Chem Assess |
|--------|-------------------------------------|---------|---------------------------|-----|-----------|------------|-----|---|------------------------|----------------------|----------------|
| 202 | 2,4,6-Trichlorophenol | 88062 | 3.5E-02 | 0.2 | 1.36 | 3.27 | 1.0 | 8.5E-05 | 9.0E-03 | 77% | Y |
| * 203 | Tris(2,3-dibromopropyl) phosphate | 126727 | 3.9E-04 | 0.0 | 874.39 | 2098.53 | 1.0 | 2.4E-05 | 2.6E-03 | 22% | Y |
| 204 | Tris(aziridinyl)-para-benz oquinone | 68768 | 1.0E-05 | 0.0 | 2.11 | 5.07 | 1.0 | 3.1E-08 | 3.3E-06 | 0% | N |
| * 205 | Urea | 57136 | 2.9E-05 | 0.0 | 0.23 | 0.55 | 1.0 | 3.0E-08 | 3.2E-06 | 0% | N |
| ** 206 | Vinyl bromide | 593602 | 4.3E-03 | 0.0 | 0.42 | 1.02 | 1.0 | 6.0E-06 | 6.3E-04 | 5% | N |
| ** 207 | Vinyl chloride | 75014 | 5.6E-03 | 0.0 | 0.24 | 0.57 | 1.0 | 5.9E-06 | 6.3E-04 | 5% | N |
| * 208 | Water | 7732185 | 1.5E-04 | 0.0 | 0.13 | 0.32 | 1.0 | 1.3E-07 | 1.4E-05 | 0% | N |
| 209 | Xylene, m- | 108383 | 5.3E-02 | 0.2 | 0.42 | 1.01 | 1.0 | 7.3E-05 | 7.7E-03 | 65% | Y |

EXHIBIT B-4

CALCULATION OF DERMAL ABSORBED DOSE FOR INORGANIC CHEMICALS IN WATER

Note: The following default exposure conditions are used to calculate exposure to chemicals in water through showering, assuming carcinogenic effects.

Given below are default values from Exhibit 3-2. For site-specific conditions, change default values to site-specific values.

Conc = 1 ppm = 0.001 mg/cm³ (default value for purpose of illustration)
SA = 18000 cm²
 t_{event} = 0.58 hr/event (35 minutes/event selected to be RME, due to high uncertainty in the value)
EV = 1 event/day
EF = 350 days/yr
ED = 30 years
BW = 70 kg
AT = 25550 days

Default conditions for screening purposes:

Compare Dermal adults (showering for 35 minutes per day) (RME value for showering) to Oral adults drinking 2 liters of water per day

$$DAD \text{ (mg/day)} = DA_{event} \times SA \times EV$$

$$\text{Oral Dose (mg/day)} = \text{Conc} \times IR \times ABS_{GI}$$

where:

IR: Ingestion rate of drinking water = 2000 (cm³/day = L/day × 1000 cm³/L)

ABS_{GI}: Absorption fraction in GI tract (chemical specific, from Exhibit 4-1)

Condition for screening: "Y" when dermal exposure exceeds 10% of oral dose value.

Refer to Appendix A for equations to evaluate DA_{event} and DAD.

The spreadsheet (INORG04_01.WK4) also provides the calculation of the ratio of the dermal dose absorbed to the total dose available from a showering scenario, assuming 5 gallons per minute as a flow rate.

All calculations are performed using the Lotus spreadsheet software, except where noted.

EXHIBIT B-4**CALCULATION OF DERMAL ABSORBED DOSE FOR
INORGANIC CHEMICALS IN WATER (continued)**

| | CHEMICAL | K _p (cm/hr) | Source of K _p (exp or default) | DA _{event} (mg/cm ² -e -event) | DAD (mg/kg -day) | ABS _{GI} (chemical specific) | Derm/ Oral (%) | Chemical to be assessed |
|----|--|---------------------------|---|--|------------------------|---|----------------------|----------------------------|
| 1 | Antimony | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 15 | 3.50 | N |
| 2 | Arsenic (arsenite) | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 95 | 0.55 | N |
| 3 | Barium | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 7 | 7.50 | N |
| 4 | Beryllium | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 0.7 | 75.00 | Y |
| 5 | Cadmium | 1.0E-03 | experimental | 5.8E-07 | 6.2E-05 | 2.5 | 21.00 | Y |
| 6 | Cadmium | 1.0E-03 | experimental | 5.8E-07 | 6.2E-05 | 5 | 10.50 | Y |
| 7 | Chromium (III) | 1.0E-03 | experimental | 5.8E-07 | 6.2E-05 | 1.3 | 40.38 | Y |
| 8 | Chromium (VI) | 2.0E-03 | experimental | 1.2E-06 | 1.2E-04 | 2.5 | 42.00 | Y |
| 9 | Copper | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 57 | 0.92 | N |
| 10 | Cyanate | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 47 | 1.12 | N |
| 11 | Manganese | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 6 | 8.75 | N |
| 12 | Mercuric chloride (other soluble salts) | 1.0E-03 | experimental | 5.8E-07 | 6.2E-05 | 7 | 7.50 | N |
| 13 | Insoluble or metallic mercury | 1.0E-03 | experimental | 5.8E-07 | 6.2E-05 | 7 | 7.50 | N |
| 14 | Nickel | 2.0E-04 | experimental | 1.2E-07 | 1.2E-05 | 4 | 2.62 | N |
| 15 | Selenium | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 30 | 1.75 | N |
| 16 | Silver | 6.0E-04 | experimental | 3.5E-07 | 3.7E-05 | 4 | 7.88 | N |
| 17 | Thallium | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 100 | 0.52 | N |
| 18 | Vanadium | 1.0E-03 | default | 5.8E-07 | 6.2E-05 | 2.6 | 20.19 | Y |
| 19 | Zinc | 6.0E-04 | experimental | 3.5E-07 | 3.7E-05 | | | highly variable |